

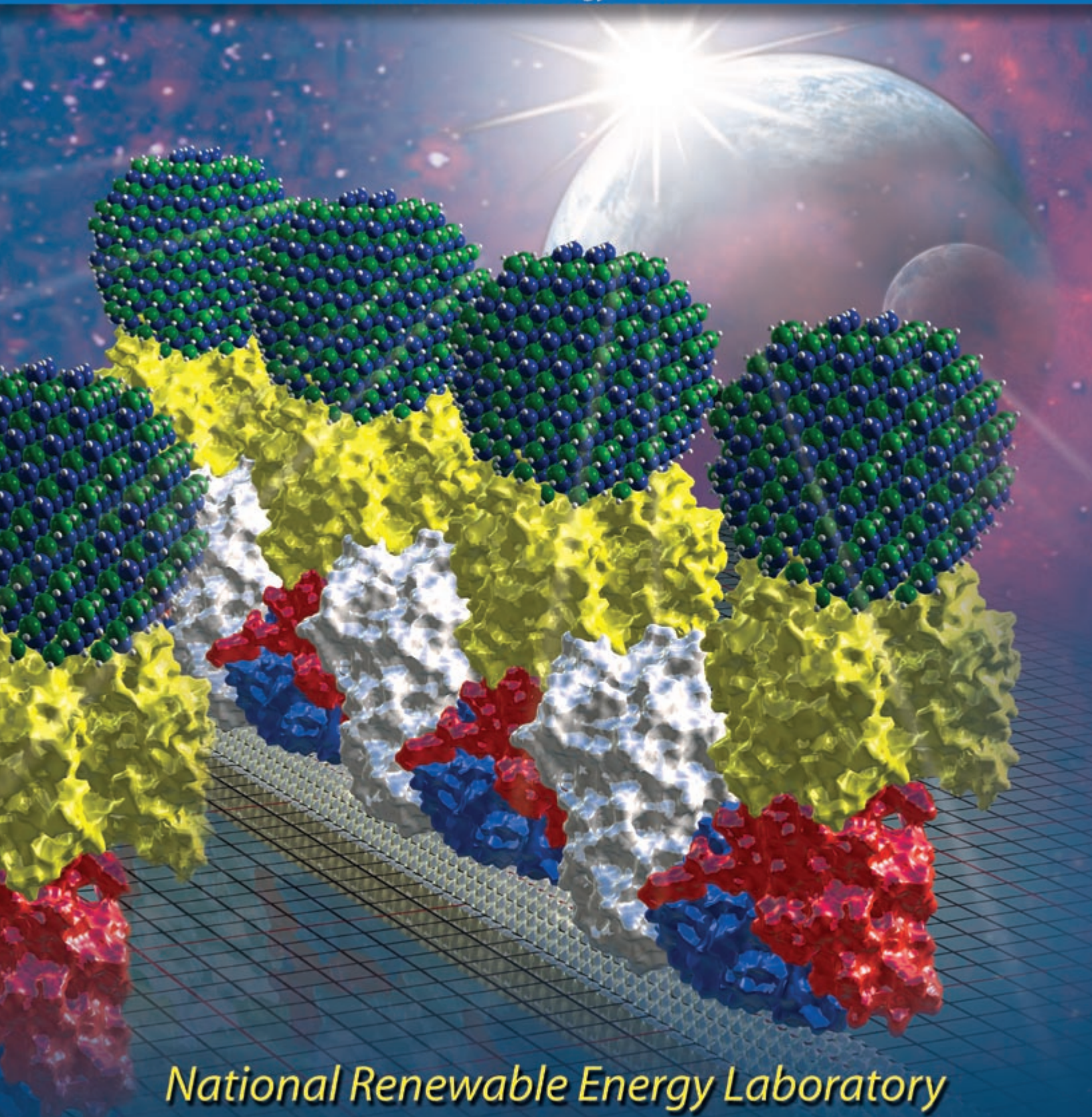


**NREL**

**National Renewable Energy Laboratory**

A national laboratory of the U.S. Department of Energy  
Office of Energy Efficiency & Renewable Energy

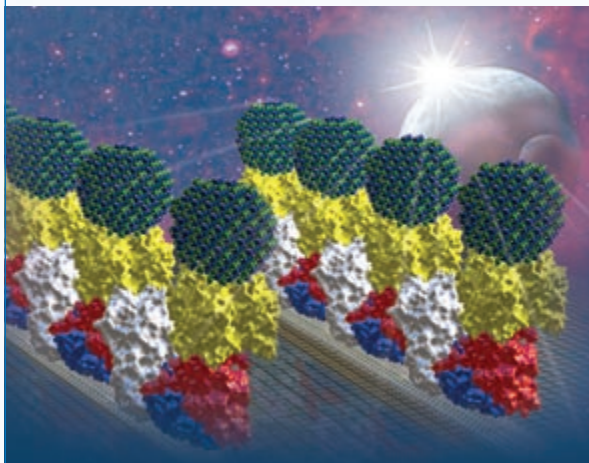
*Innovation for Our Energy Future*



*National Renewable Energy Laboratory*  
***2004 Research Review***



## feature



### 8 NREL Nanoscience & Nanotechnology

**Aligning Quantum Dots.** Quantum dots will be important for a variety of renewable energy technologies in the 21st century, especially for a new generation of photovoltaic technologies. Properly aligned quantum dots could result in highly efficient, low-cost devices. The cover shows the use of cellulosome proteins for this alignment—a unique technique being explored by NREL scientists and described in the feature article.

## departments

**1 Perspective** Meeting our mission requires an R&D management philosophy that carefully shepherds research from inception to the development of technologies that will benefit the nation.

**2 NREL in Focus** 2004 news stories include the retirement of one director and the arrival of another, breaking ground for a new research facility, NREL becoming a hydrogen center of excellence, ISO certification for calibrating reference cells, and recognition of an NREL research fellow for high-citation impact.



**4 Awards & Honors** During 2004, NREL was honored with two R&D 100 Awards, three regional technology transfer awards, a solar energy award, a Secretary of Energy Gold Award, and the naming of a new science society fellow.



## articles

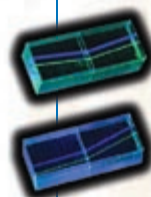
**18 The Story of ADAM** With their Advanced Automotive Manikin (ADAM), NREL researchers have created a tool that will help in the testing and design of ancillary automotive systems, making cars and light trucks more comfortable and energy efficient.



**22 Harvesting the Ocean Wind** Winds coursing the "deep" waters off the shores of New England could provide that region with 100 MW or more of clean wind-generated electric capacity. NREL engineers are tackling the technical challenges to designing and building deep-water wind turbines.



**24 Research Update** In other research areas, NREL scientists are the first to achieve negative refraction of light using natural materials, help to develop concepts that will enhance the production of geothermal power, and perfect new ways to measure minority-carrier lifetimes in photovoltaic and semiconductor materials.



**The NREL Research Review.** The National Renewable Energy Laboratory is operated by Midwest Research Institute and Battelle for the Department of Energy's Office of Energy Efficiency and Renewable Energy. NREL is the nation's primary national laboratory for renewable energy and energy efficiency research and development. The *Research Review* is published yearly and describes the Laboratory's accomplishments in science and technology to a wide audience. The purpose is not simply to describe the progress being made, but also to show the promise and value of NREL's R&D to people, industry, the nation, and the world.



# Perspective

## Science and Technology: From Innovation and Knowledge to Implementation

Our mission at NREL is not simply to perform R&D on renewable energy and energy efficiency technologies, but also to make sure that the innovation and knowledge we generate is taken through implementation to address the nation's energy, environmental, and economic goals. The path from idea to fruition is challenging, and our R&D can face many obstacles on the way.

To help ensure success, we have a management paradigm that takes science and technology from initial concept through a process that enables the concept to reach its final goal. This process includes strategy and plans, hypothesis and verification, delivering R&D accomplishments in technology development, and forming and nurturing partnerships—all ending in the development of a technology that is ready to benefit the nation and the world.

One of our principal measures of success is to win R&D 100 awards, which are presented by *R&D Magazine* to the 100 most technologically significant products and processes of the year. The awards represent an affirmation that our research ideas are being used in the real world to help meet America's needs and that we are meeting our mission. Since 1979, NREL has won 37 of these awards, 31 since 1991.

In 2004, NREL won two more R&D 100 awards (see stories on pages 4–6)—one for lightweight, flexible, copper indium gallium diselenide PV modules; and the other for enzymatic hydrolysis of biomass

cellulose to sugars. Both technologies are representative of our R&D management paradigm. Consider the enzymatic hydrolysis technology, which has a long history at NREL. One of the Laboratory's original programs involved the development of technologies to produce alternative fuels from biomass, to relieve America's growing dependence on imported oil. From the beginning, NREL realized that, in the long term, cellulosic biomass presented the largest resource for such alternative fuels. Moreover, enzymatic hydrolysis of cellulose represented the preferred pathway for lowering the cost to where fuels derived from cellulosic biomass could not only be competitive with other alternative fuels but also with petroleum.

NREL subsequently laid out a long-term strategy to develop the enzymatic technology base and meet the cost goals, emphasizing the emerging fields of genetic and protein engineering and enzyme production. The R&D approach under this strategy involved basic research to discover appropriate microorganisms, engineer the variations, and produce those variations. It also involved a parallel effort in applied research and engineering to integrate the microorganisms into hydrolysis and fermentation processes. Once the technology was sufficiently proven, NREL sought partners who could better engineer enzymes and who could efficiently produce the enzymes in quantity. NREL reached a partnership



**Dr. Stanley R. Bull, Associate  
Director, Science & Technology**

agreement with two of the best in the world—Genencor International and Novozymes Biotech Inc. This NREL/Genencor/Novozymes partnership quickly resulted in technological

advances that cut by 20-fold the cost of enzymatic hydrolysis. This is now becoming a “real-world” technology that will help open America's vast biomass resources for the economic production of not only alternative fuels, but also chemicals, plastics, and many other products—while offsetting the use of petroleum.

Today, with its research in nanoscience and nanotechnology (see story on pages 8–17), NREL is facing a situation analogous to that which it faced with enzymatic hydrolysis a decade or so ago. Some of our R&D is still in the basic phase, with hypotheses being formed and tested. But in other avenues of exploration, we are performing applied research and are entering into collaborations and partnerships with universities, institutes, and companies. Nanotechnology is an extremely promising area for energy research and development. If the R&D is managed following our established paradigm, it will lead to a new frontier of energy solutions, which is so important for the nation and the world. As with past and present successes, we are confident that the nanoscience and nanotechnology being researched at the Laboratory today will become the real-world technologies of tomorrow.

This is not just our belief—it is our mission.

# NREL In Focus



Admiral Richard H. Truly



Dr. Dan E. Arvizu

## Passing the Torch

NREL welcomed new director Dr. Dan E. Arvizu January 15, 2005, and honored the accomplishments of retiring director Richard H. Truly.

In his seven years at NREL's helm, Truly established the National Bioenergy Center at NREL; brought the hydrogen systems integration function to the Laboratory; secured a key for NREL in the Center of Excellence for exploratory research in hydrogen storage; began construction of the Science and Technology Facility, NREL's first major new building in more than a decade; and created Sustainable NREL, a campus-wide effort to incorporate sustainable energy practices throughout the workplace. Streamlining management systems was another priority that bore significant benefits and resulted in more funds directed toward laboratory R&D.

"Science and engineering have a magical quality about them, in that they are all about imagining a future that gets created by those lucky enough to have their ladle in the broth," Truly said in announcing his retirement. "I feel a deep privilege to have been a small part of NREL's successes over these years."

Dan Arvizu is NREL's eighth director in its 27-year history. In addition to his

NREL appointment, Arvizu joins Midwest Research Institute (MRI) executive management and assumes a senior vice president position. NREL is operated for the Department of Energy by MRI and Battelle.

Prior to joining NREL, Arvizu held prominent positions at CH2M Hill from 1998 to 2004. Most recently, he served as senior vice president and chief technology officer overseeing technology development and acquisitions for seven major business groups, with more than \$2.5 billion in annual revenue. Arvizu spent more than 20 years managing energy research programs at Sandia National Laboratories, including supervising the Photovoltaic Cell Research and Concentrator Division. Arvizu was credited with expanding the laboratory's technology transfer efforts, first as director of the Technology Commercialization Center and later as director of the Advanced Energy Technology and Policy Center.

In 2004, Arvizu was appointed by President George W. Bush to serve on the National Science Board, which is the governing board of the National Science Foundation. He also serves on several university advisory boards, on the board of directors of the Hispanic Engineers National Achievement Awards Corp., and on the board of advisors for the Greater Denver Metro Area Salvation Army.

Arvizu has served on numerous other boards and advisory committees, including the National Coal Council, the Army Science Board, the National Academies of Sciences and Engineering, the G8 International Renewable Energy Task Force, and the Council on Competitiveness.

## Breaking Ground for New Facility

NREL broke ground in July to signal the start of construction of the new Science and Technology Facility (S&TF). The 71,000 square foot, energy-efficient building will include laboratory space, offices, and a lobby. Situated at the foot of South Table Mesa on NREL's main campus, the S&TF will be connected by an elevated bridge with the Solar Energy Research Facility. The new building will expand NREL's capabilities in photovoltaics, hydrogen, solid-state lighting, basic sciences, and nanotechnology and will reduce barriers and time delays associated with transferring technology from R&D to industry.

National leaders present at the groundbreaking included U.S. Senator Wayne Allard and Congressman Bob Beauprez, who extolled NREL as an asset to Colorado and the nation, and praised the project as a beneficial new resource for ensuring U.S. energy security.

"This new facility will . . . hasten the day when we reach our goal of providing . . . clean, affordable energy solutions that can be used by all Americans," said David Garman, DOE's acting under secretary for energy, science, and the environment and assistant secretary for energy efficiency and renewable energy.

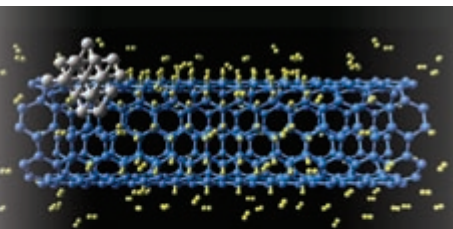
**NREL's Science and Technology Facility, which is scheduled for completion in 2006, will be NREL's first major new facility in a decade. The S&TF will be used for R&D in photovoltaics, hydrogen, solid-state lighting, basic sciences, and nanotechnology.**





Construction began in earnest in early 2005, with completion expected in late 2006.

The value of the construction subcontract is nearly \$18 million. The total value of the project, including equipment and furnishings, is approximately \$28 million. The M.A. Mortenson Company signed the contract to build NREL's first major new facility in a decade.



An important concept for hydrogen storage that NREL is exploring is a single-wall carbon nanotubes (blue), shown here with hydrogen (yellow) diffusing to the lattice of the nanotube in the presence of a catalyst (silver).

## NREL Named to Hydrogen Center of Excellence

NREL was named by DOE to play a key role in one of three "Centers of Excellence" for exploratory research in hydrogen storage and nanostructured carbon-containing materials. The other centers—to study chemical and metal hydrides for hydrogen storage—have Los Alamos National Laboratory and Sandia National Laboratories in key roles. Each center will lead R&D on different material systems to address major technical barriers to storing hydrogen on-board cars, vans, and light trucks. The goal is to develop systems that will store enough hydrogen to enable a driving range greater than 300 miles without impacting cargo or passenger space.

NREL is in the Center of Excellence for carbon-based materials and will lead research on carbon nanotubes, nanofibers, and aerogels, alkali metal intercalated carbons; and other novel carbon-based materials. In this endeavor, it will partner with industry (Air Products and Chemicals Inc.); universities (California Institute of Technology, Duke University, Penn State University, Rice University, University of Michigan, University of North Carolina, and

University of Pennsylvania); and other national laboratories (Lawrence Livermore National Laboratory, National Institutes of Standards and Technology, and Oak Ridge National Laboratory).

## NREL Wins ISO Certification

NREL's National Center for Photovoltaics received ISO (International Organization for Standardization) 17025 accreditation in recognition of the Center's stringent standards in calibrating secondary photovoltaic reference cells. These reference cells are used by calibration and testing laboratories and by PV manufacturers, who can now be assured that their calibrations and measurements are traceable, via NREL's certified reference cells, to national and international standards.

The ISO 17025 accreditation was granted by the American Association for Laboratory Accreditation. Only one other laboratory in the world—the European Solar Test Installation—has the same accreditation, according to NREL scientist Keith Emery. Other labs have accreditation in similar types of calibration.

ISO 17025 accreditation is awarded in many industries, each with its own standards. It is a recognition sought by testing and calibration laboratories, inspection bodies, proficiency testing providers, and reference material producers. To win such accreditation, a laboratory must have a quality system at three levels of staff: top management, supervisors, and operating personnel. Quality procedures must be described in a manual. The laboratory must have a policy and procedures for corrective actions in the event of non-conforming data results.

## NREL Theorist Recognized for High-Citation Impact

Dr. Alex Zunger, NREL research fellow, is the co-author of a paper that has had the fifth-highest citation impact in the *Physical Review* during the past 110 years, according to a recent analysis of papers appearing in the journal.

The analysis, performed by Sydney Redner of Boston University, includes more than 3 million citations from more than 329,000 manuscripts appearing in the prestigious physics journal from 1893 through 2003.

Citation impact is based on the number of citations to a publication times the average age of these citations. Such a measure emphasizes publications that have influence over an extended period of time.

Zunger's achievement is based on his work with John Perdew on "Self-interaction Correction to the Density Functional Approximation for Many-Electron Systems" published in *Phys. Rev. B* 23, 5048 (1981). Their paper established a fundamental treatment of Walter Kohn's and Lu Sham's celebrated "Density Functional Theory" (ranked number one in Redner's analysis). This opened up the field of using the quantum theory of Kohn and Sham to predict optical, structural, and energetic properties of many molecules and solids.

Zunger's Solid State Theory group at NREL has used this method during the past 20 years to predict and analyze the properties of PV materials and to study spontaneous ordering, alloy bowing, and, more recently, the properties of nanostructures.

Dr. Zunger has been with NREL for 25 years and has been a research fellow at the Laboratory since 1991. He has authored and co-authored more than 400 journal articles. According to a recent study by the Institute of Scientific Information, other papers by Zunger place him in 39th place (of 50,000 physicists reviewed) in terms of citations by all physics journals in the years 1987–1997.



NREL research fellow Alex Zunger co-authored one of the highest-ranked papers (in terms of citation impact) ever published in *Physical Review*.



# Awards & Honors

## R&D 100 Awards

Every year, *R&D Magazine* holds an international competition to select the 100 most significant technological advances of the year. Winning one of these hotly contested awards—often referred to as the Academy Awards of technology—has become a widely recognized honor for the winning technology and the R&D that went into its development. Since NREL first opened its doors as the Solar Energy Research Institute in 1979, the Laboratory—often in collaboration with research partners—has won 37 of these awards, 31 of them since 1991. In 2004, NREL was honored with two more R&D 100 awards.

## Making Fuels and Chemicals from Sugar

NREL and its partners—Genencor International and Novozymes Biotech Inc.—developed a technology that uses enzymatic hydrolysis to inexpensively break down the cellulose fraction of lignocellulosic biomass to sugars. The sugars can then serve as platform chemicals from which to derive ethanol fuel, other fuels, chemicals, and many other products—all sustainably. Such a concept, known as biorefining, is analogous to petroleum refining except it is based on renewable feedstocks and could help America offset its use of petroleum-derived fuels and chemicals.

Before the advent of our technology, the process for breaking down cellulose to sugars was too expensive to compete with the technology used to

break down starch in corn kernels to sugars; or to compete with breaking down hydrocarbons in petroleum for the production of the fuels, chemicals, and products that help run our modern economy.

Lignocellulosic biomass consists of cellulose, hemicellulose, and lignin, with cellulose constituting up to 50% of the total mass. Like starch and sugar, hemicellulose and cellulose are carbohydrates (compounds of carbon, hydrogen, and oxygen). The sugars of which they are made are linked together in long chains called polysaccharides, which form the structural portion of plant cell walls. Unraveling these complex structures is the key to economic biorefining.

Cellulose microfibrils consist of a crystalline structure of thousands of strands, each of which contains hundreds of glucose sugar molecules. These microfibrils are wrapped in a sheath of hemicellulose and lignin, which protects the cellulose from microbial attack. Hemicellulose is relatively easy to break down into its component sugars using heat, pressure, and dilute acid. This “dilute acid hydrolysis” pretreatment step also disrupts the hemicellulose/lignin sheath around the cellulose, making the cellulose accessible to further hydrolysis.

To hydrolyze the cellulose, NREL and its partners developed a technology that employs a cocktail of three types of cellulase enzymes—endoglucanase, exoglucanase, and betaglucosidase. In consort, these enzymes break cellulose chains in two, exposing the ends of the chains, and then break down these chains into units of cellobiose (a dimeric sugar comprised of two





glucose molecules). They then split the cellobiose molecule into two separate glucose molecules, making them available for processing into fuels or chemicals.

Until the advent of our breakthrough technology, other methods of hydrolyzing cellulose to sugars—including strong acid hydrolysis and older versions of enzymatic hydrolysis—were inefficient, expensive, and had low sugar yields. Enzymatic hydrolysis was also too expensive, but it had great potential. The strategy to take advantage of this potential was twofold: improve the pretreatment (i.e., the dilute acid hydrolysis) process and reduce the cost of the enzymes. Reducing the cost of the enzymes also followed a twofold strategy: engineer better enzymes, so that less enzyme is needed per gallon unit of sugar output; and optimize the enzyme-production system. The task of improving the pretreatment fell to NREL, while reducing the cost of the enzymes became the task of Genencor and Novozymes (working separately on their respective proprietary strains to produce more efficient cellulase systems and to improve the economics of their proprietary production methods). NREL also validated and verified technical improvements at each stage of development.

As a result, NREL and its partners developed a technology that is efficient, has high sugar yields, and has already dropped the cost of cellulose hydrolysis by 20-fold. Moreover, this technology holds the promise of decreasing the cost by as much as another order of magnitude, and maybe more.

One of the reasons for developing this technology is to produce inexpensive ethanol fuel from lignocellulosic biomass. The United States has enough

of this resource to sustainably make as much as 30 to 45 billion gallons of ethanol per year. This would not only significantly offset the nation's consumption of gasoline (which stands at about 135 billion gallons today), but it would also lead to large offsets of greenhouse-gas emissions as the ethanol displaces our use of petroleum. Ethanol derived from lignocellulosic biomass can use the lignin portion to produce the heat and electricity required to run the process to make it. The use of lignin thus offsets energy that would otherwise be conventionally obtained from fossil fuels. This, along with the fact that burning ethanol produces less net CO<sub>2</sub> emissions as a result of re-assimilation of CO<sub>2</sub> into plant matter via the carbon cycle (growing biomass absorbs CO<sub>2</sub>), enables the entire "plant to wheels" process of lignocellulosic production of fuel ethanol to actually have negative greenhouse gas emissions relative to the "oil well to wheels" process for gasoline. The end result is a net offset of up to 600 g of CO<sub>2</sub> per mile when lignocellulosic ethanol is used for transportation in place of petroleum.

But producing ethanol fuel is just the beginning. Using different microbes and processing techniques, we can build biorefineries with which to derive many other products, including plastics, fibers, textiles, polymers, films, lubricants, adhesives, cements, solvents, chemical intermediates, photographic chemicals, cleaning agents, coatings and paints, fillers and insulation, cosmetics and personal-care products, pharmaceuticals and medical and dental products, other alcohols,

antifreeze, softening agents, sweeteners, dyes and perfumes, insecticides, food additives, and much more. Our technology, therefore, could help biorefineries begin to play a major role in America's economy.

## Portable Solar Electricity

Thanks to Global Solar and its partners at ITN Energy Systems and NREL, the world now has its first portable, flexible PV systems made from copper indium gallium selenide (CIGS)—for use in mobile applications. These PV systems can provide from 12 W to 56 W of power, be folded into sizes as small as a 9 x 12 envelope, and be easily stowed in a small backpack. In addition, they are light enough to be carried over long distances, and can be connected together, when needed, to provide as much as 2.8 kW of power. One line of products using this technology is flexible enough to be rolled up to a size comparable to modern, lightweight, self-inflating mattresses used in backpacking.

The U.S. Army is already using these new systems in applications where both weight and space are at a premium—such as for scouts, forward field officers, special operations units, and forward communication units. For the military, the flexible CIGS modules can also provide portable power in the field without the drawback of the heat signature of diesel or gasoline generators.

Many of the features that make this technology so attractive to the military also make it appealing to a wide range of other applications. This

**NREL researchers (left) collaborated with researchers from Genencor International (middle) and Novozymes Biotech Inc. (right) to develop an award-winning technology that enzymatically reduces cellulose to sugars. Only a few members and leaders of these large research teams are present in the photos.**





CIGS technology can provide reliable power for hikers, campers, and boaters; police; portable electronics, such as cell phones, satellite phones, GPS units, computers, radios, and MP3 players; survival kits; battery chargers; and more.

The CIGS systems are not the first portable PV systems available. Systems based on amorphous silicon technology have been on the market for a few years. But the new CIGS portable PV technology has many advantages over these systems. Compared to them, for example, the CIGS systems:

- Are lighter, more flexible, and portable
- Are more efficient and reliable
- Have two to three times the power-to-weight ratio
- Have more than five times the power-to-volume ratio
- Cost less
- Are inherently self-repairing due to the natural tendency of copper atoms in the CIGS material to spread into damaged areas, thereby repairing the crystal structure. In fact, CIGS modules can even take a bullet hole and continue to operate.

Another advantage of the CIGS technology is that it is extremely versatile. Modules can be fabricated on a variety of substrates—flexible, rigid, or substrates that can conform to many surfaces. As such, the CIGS systems can be included on all kinds of structures such as signs, bus shelters, sun roofs, or awnings; or they can be integrated into building applications and be used on metal roofs, as roof shingles, or in architectural fabrics or facades.

From 1994 through 2004 worldwide PV module sales increased more than 15-fold—from less than 70 MW per year

to more than 1.1 GW per year. And the annual market for the sale and installation of PV systems is fast approaching \$10 billion. The great majority of this market belongs to silicon PV technology, especially crystalline silicon. The advent of flexible CIGS technology is significant for at least two reasons. First, this technology is opening up a whole new category of applications for photovoltaics. Second, but equally important is the arrival of this valuable thin-film material on the commercial scene. It has a great potential, especially as it gains a larger share of the market, to reduce the cost of PV electricity and thus augment the phenomenal growth of the PV market.

## Other Awards & Honors

### Technology Transfer Awards

NREL was honored with three awards from the Mid-Continent Region of the Federal Laboratory Consortium (FLC) for Technology Transfer. The awards were presented at a September banquet on South Padre Island, Texas.

Two of the awards were for Notable Technology Development. The first of these recognized the work that the Vehicle Ancillary Loads Reduction Team performed for the Thermal Comfort Project. Team members Rob Farrington, John Rugh, Jason Lustbader, and Charlie King developed tools to analyze and improve the efficiency of climate control in vehicles. Their work has resulted

in the development of the ADvanced Automotive Manikin (ADAM), the world's most advanced thermal comfort manikin. Using computer models that simulate human physical and psychological responses, it mimics human responses such as sweating and breathing. ADAM is designed not only to determine how hot or cold an occupant is, but also to predict how the occupant will feel.

The second award recognized the Advanced Petroleum-Based Fuels (APBF) Project, whose team members include Wendy Clark, Shawn Whitacre, Theresa Alleman, and Matt Thornton. The award commended their efforts in forming industrial partnerships, with the ultimate aim of reducing transportation-related petrochemical use and emissions. Project partners include vehicle manufacturers, equipment suppliers, and fuel providers. The APBF team brings value in the form of state-of-the-art laboratories and research, and patented technologies available for licensing.

Both projects are managed by the Laboratory's Center for Transportation Technologies and Systems.

Also honored by the FLC was Lawrence "Marty" Murphy, manager of NREL's Enterprise Development Programs. Murphy received a Distinguished Service Award for his leadership during the past nine years in building and promoting NREL's Enterprise Development Program and Industry Growth Venture Forums, which encourage the creation and growth of clean, efficient, and renewable energy companies. In the past few years, these activities have resulted in at least \$5 million in private capital and \$5 million in state and local funds for clean-energy commercialization, and more than 1,000 jobs created in successful clean-energy companies.



A Global Solar team (right), worked with teams from NREL (left) and ITN Energy Systems to develop lightweight, flexible, portable PV modules (above).





## Steve Kelley Elected IAWS Fellow

In recognition of his valuable contributions to the fields of wood chemistry and technology, Principal Scientist Steve Kelley was elected a fellow of the International Academy of Wood Science (IAWS).

Since he joined NREL in 1992, Kelley's research has primarily focused on two areas: developing value-added products from biomass, and applying novel analytical tools for characterizing biomass and natural polymers.

Kelley has worked on developing phenolic resins from wood and bark, to replace petrochemical adhesives used to make wood products such as plywood. He has also worked to develop technology for making chemicals, monomers, and plastics from biomass rather than from petrochemicals.

"Cellulose, hemicellulose, and lignin in biomass are polymers to begin with," Kelley explains. "In the biorefinery approach that NREL is developing, we use chemical or biological techniques to break down the polymers to building blocks that can be refined and used for value-added applications. We have also looked at isolating and using the polymers in their original form."

Kelley was a key player in developing NREL's rapid biomass analysis technology, for which he and fellow researchers earned a prestigious R&D 100 Award in 2000. Combining near-infrared spectrometry with sophisticated multivariate analysis, the technology allows virtually instantaneous, nondestructive analysis of biomass, eliminating the need for expensive laboratory analysis that might take weeks. Kelley has taken this technology beyond its initial application for chemical analysis, extending its capabilities to determine mechanical properties and wood decay, and to evaluate wood composites. For example, it can be used to assess the dry strength of lumber that could be made from a tree while the tree is still standing in the forest.

Kelley has been the NREL lead on a series of projects designed to demonstrate the utility of these rapid analysis tools for understanding the effects of process variables on the chemical and physical properties of bio-based materials. He holds a B.S. in wood science from Oregon State University; an

M.S. in forestry and wood science from the University of Wisconsin, Madison; and a Ph.D. in polymer chemistry from Virginia Tech. He has co-authored 65 publications and has 15 patents and submitted applications.

## Women in Solar Energy Award

Cecile Warner, an NREL staff member for more than 25 years, received the 2004 Women in Solar Energy Award from the American Solar Energy Society. She was praised for outstanding and sustained contributions to solar photovoltaics, particularly for her public outreach efforts.



**Cecile Warner stands on the mall in the nation's capitol, where crowds of people flock to see solar-powered homes designed by teams of college students for the U.S. Solar Decathlon.**

In 2002, Warner led the Laboratory in developing and managing the highly acclaimed U.S. Solar Decathlon for the U.S. Department of Energy. The Solar Decathlon is a competition in which teams of college and university students compete to design the most attractive, effective, and efficient solar-powered house. She also served as director of the Laboratory's

Center for Renewable Energy Resources from 1996–2000; and was project director of Sunrayce 93, a university competition of solar cars. Warner was elected to the Board of Directors of the American Solar Energy Society in 2000. She holds a B.S. and M.S. in mechanical engineering.

## Truly Receives Energy Secretary's Gold Award

Former Secretary of Energy Spencer Abraham presented the Secretary's Gold Award to NREL Director Richard Truly and seven other current and former directors of DOE national laboratories. The award is DOE's highest honorary award and includes a plaque with citation, a medallion, and a rosette.

"I'm proud to recognize the people whose hard work and dedication contribute so much to the Department of Energy's vital missions," Abraham said. "Our world-class laboratories are a marvelous resource and have made far-reaching contributions—not only to the Department of Energy, but to our nation and, indeed, the world. The incredible work done in the laboratories is made possible by the strong, steady, and responsible leadership of these directors."

Truly was recognized for his superior leadership as director of NREL and for his vision and perseverance in helping transform NREL into the premier national institution in its field.

Secretary Abraham presented the awards at an October 25 luncheon at the Woodrow Wilson International Center for Scholars in Washington, D.C.

**The Secretary's Gold Award plaque was presented to NREL director Richard Truly by former DOE Secretary Spencer Abraham.**







# NREL Nanoscience & Nanotechnology

Meeting 21st Century  
Energy Challenges

Many futurists, scientists, and technologists believe that nanotechnology in the 21st century could prove to be as socially transformative as running water, antibiotics, plastics, or semiconductors have been. Nanotechnology will have a crucial impact on everything from cars, health, and security to computers and materials science. Serious projections for it include building materials that can sense weather and change properties accordingly, lightweight materials far more durable than steel and hundreds of times stronger, computers that are orders of magnitude faster than today's, and nanoscale biosensors that can be injected into blood streams to diagnose and treat illnesses.

At NREL, we see the 21st century also as a century of new energy concepts and nanotechnology as a technology that will enable sustainable, benign, efficient, and inexpensive energy. In fact, when applied to energy, the impact of nanotechnology may turn out to be as great as that brought about by civilization's turn to fossil fuels, which resulted in the industrial revolution. To put this in perspective, today the world consumes about 13 terawatt-years (TW-yr) of energy per year. (A terawatt is  $10^{12}$  W.) But according to the DOE's Basic Energy Sciences Advisory Committee, the world's energy consumption will more



than double by 2050. And papers from Hoffert et al. published in the journal *Nature* show that, if we are to meet this demand while stabilizing the CO<sub>2</sub> in the atmosphere at a reasonable level—such as 550 parts per million, or twice the pre-industrial level—at least 100% of this new energy would have to come from non-CO<sub>2</sub> generating sources. This is a daunting challenge that will take a major effort and important breakthroughs in energy technology and science. Nanotechnology will help meet this challenge.

Nanotechnology deals with materials and phenomena on the scale of 1 billionth (10<sup>-9</sup>) to several tens of billions of a meter. This is larger than the atomic scale, smaller than the bulk scale, and about the size of some molecules, including DNA and proteins. But the nanoscale is not simply a move toward miniaturization. It is a scale at which properties are qualitatively different from those of bulk materials. This includes electrical, material, and optical properties. Because of these properties and because of new techniques, we can design and construct new materials and systems with attributes and capabilities not found in bulk material or in nature.

## NREL's Early Start

It is because of these qualitatively different properties and their applications to renewable energy and energy efficiency that NREL has long been studying nanotechnology. In its early efforts, NREL explored specific nanoscale components and materials, how to make them, their characteristics and properties, the mechanisms underlying those properties, and how to understand those properties and predict others.

For example, in 1983, shortly after the Laboratory first opened its doors, NREL began making and studying colloidal quantum dots (QDs). NREL researchers were among the first to report on the quantization effects of nanosized semiconductor particles—a phenomenon whereby emission and absorption spectra vary dramatically with the size of the nanoparticle (see sidebar “Quantum Confinement: Shifting Toward the Blue”).

Starting in 1991, NREL's Solid-State Theory Group began fundamental explorations of QDs, developing a theory that enables them to model optical and electronic properties of neutral and charged QDs and QD arrays. NREL also began its study of single-wall carbon nanotubes in 1993, the same year their existence was discovered, and of nanoparticle precursors in 1995.

**Nanoparticle Precursors.** Nanoparticle precursors are typically metal or semiconductor material crystalline structures less than 20 nm in diameter and that are used to form a precursor state for a macroscopic device. In the process of forming the macroscopic device, the nanoscale nature of the starting material is altered or destroyed. Although nanoparticle precursors do not generally exhibit

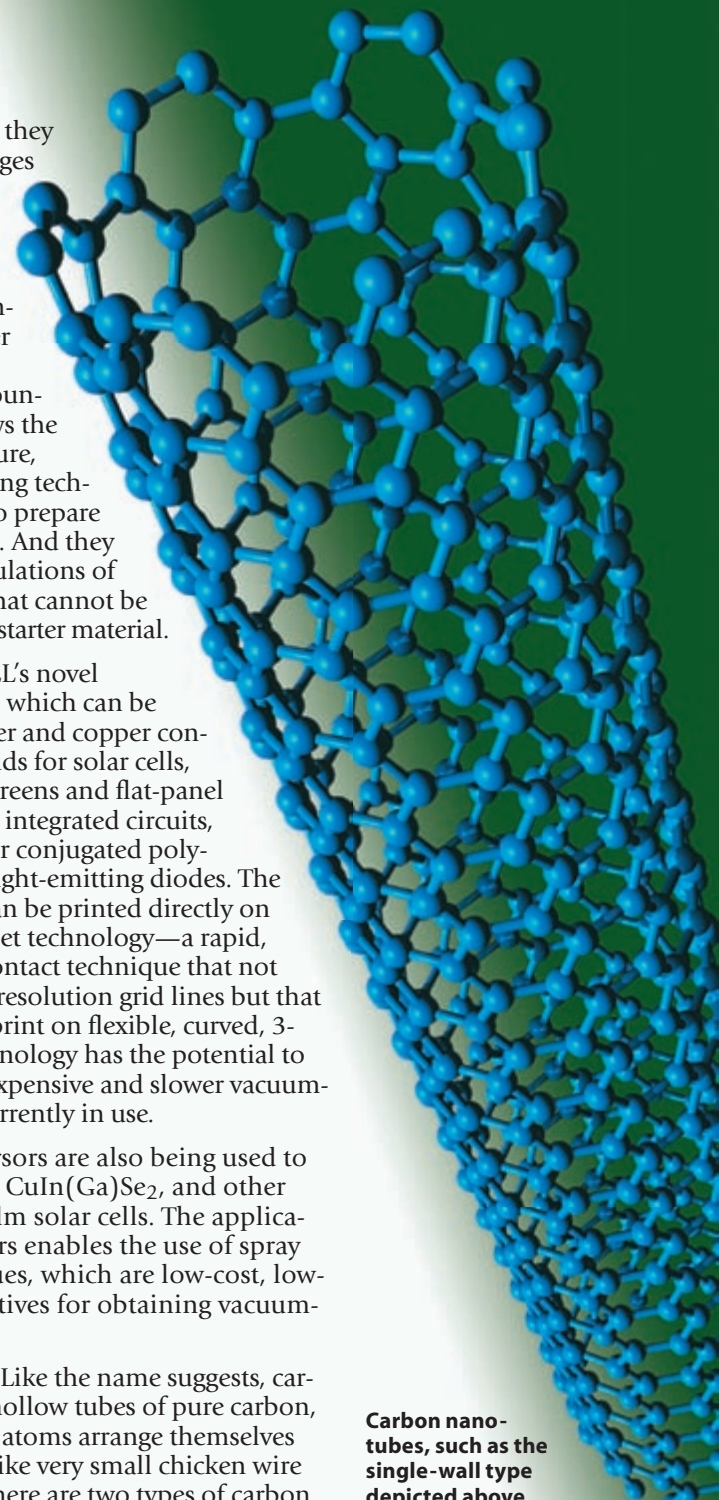
quantization effects, they have several advantages over other starting materials. They can be easily and inexpensively prepared using colloidal chemistry. They have lower melting points than their macroscopic counterparts, which allows the use of low-temperature, inexpensive processing techniques with which to prepare macroscopic devices. And they allow versatile formulations of solutions and inks that cannot be obtained with larger starter material.

One example is NREL's novel organometallic inks, which can be used to produce silver and copper contacts and metallic grids for solar cells, contacts for touch screens and flat-panel displays, busbars for integrated circuits, and metallic grids for conjugated polymer solar cells and light-emitting diodes. The grids and contacts can be printed directly on the device using inkjet technology—a rapid, atmospheric, non-contact technique that not only produces high-resolution grid lines but that also can be used to print on flexible, curved, 3-D surfaces. This technology has the potential to supplant the more expensive and slower vacuum-based technology currently in use.

Nanoparticle precursors are also being used to make films of CdTe, CuIn(Ga)Se<sub>2</sub>, and other materials for thin-film solar cells. The application of the precursors enables the use of spray deposition techniques, which are low-cost, low-temperature alternatives for obtaining vacuum-quality materials.

**Carbon Nanotubes.** Like the name suggests, carbon nanotubes are hollow tubes of pure carbon, in which the carbon atoms arrange themselves in hexagonal rings, like very small chicken wire rolled into a tube. There are two types of carbon nanotubes: single-wall nanotubes (SWNTs), comprised of a single shell of carbon atoms, approximately 1–2 nm in diameter and several microns long; and multi-wall nanotubes (MWNTs), comprised of multiple concentric nested tubes, with an outside diameter of several tens of nanometers.

NREL is one of the few labs to use all four of the known major methods for synthesizing nanotubes. The first one used at NREL was the same method used to discover SWNTs: arc-discharge. Subsequently, NREL developed a laser vaporization technique in which a graphite target is irradiated with laser pulses. The pulses evaporate the graphite target to produce a variety of reactive carbon intermediate structures that, when quenched



Carbon nanotubes, such as the single-wall type depicted above, exhibit properties that make them attractive for a wide variety of applications. On the opposite page are quantum dots being aligned using a cellulosome polymer; the De-Broglie wavelength equation for matter waves; a  $\pi$ -conjugated polymer structure; and a C<sub>60</sub> “buckyball.”



To exist, an electron in a confined space (such as in a spherical quantum dot) must have an associated wavelength that is equal to the inside circumference of the confining space or a whole number fraction thereof ( $\frac{1}{2}$ ,  $\frac{1}{3}$ ,  $\frac{1}{4}$ , etc.). The smaller the dot, the shorter the wavelength that fits, the higher the energy of the electron. Hence, the absorption and emission spectra shift to the blue (higher energy) for smaller dots.

in the presence of the appropriate catalyst, form the nanotubes. The diameter of the SWNTs can be manipulated by controlling the pulse power of the laser—the higher the pulse power, the smaller the carbon fragments and the smaller the diameter of the tubes. NREL has also developed chemical vapor deposition methods to form SWNTs using methane as a feed gas. This process, though not as controllable as the laser-based one, promises to be amenable to low-cost, large-scale manufacture of nanotubes. Recently, NREL developed a hot-wire chemical vapor deposition technique, in which a hot wire filament in a vacuum chamber is heated in a carbon-bearing gas, such as methane. As the gas decomposes, it frees the carbon atoms, which recombine to form multi-wall nanotubes.

Carbon nanotubes have interesting properties that make them valuable for a variety of applications. For example, they have extremely high tensile strength and could be used in composites for making armor, space crafts, or lightweight, resilient cars (important for energy-efficient transportation). Multi-wall nanotubes have interesting field emission characteristics, prodigiously emitting electrons at low voltage from their tips; this gives them great potential for use in solid-state lighting and flat-plate displays.

Because SWNTs have small diameters, typically less than 2–3 nm, quantum effects are readily apparent. For example, electrons in a SWNT can maintain their quantum state and travel ballistically along the nanotube, electrons and photons are strongly coupled, and exciton binding energies exceeding 1 eV have been predicted. In addition, SWNTs can be made with either semiconductor or metallic properties, depending on how the two-dimensional sheets of graphite are rolled up. The semiconductor variants exhibit strong photoluminescence. These properties make SWNTs ideal candidates for wires that carry high current and for applications in which highly conductive and high-surface materials

are required, such as in fuel cells, ultracapacitors, and organic photovoltaics. They are also strong candidates for supports for other nanoscale catalysts. Nanotubes can also be used as interconnects in highly efficient electronic switches, for photoactive media in transistors or solar cells, and as conduits for transferring charge carriers between quantum dots.

One characteristic of great interest to NREL is the ability of SWNTs to reversibly store lithium ions and hydrogen gas. This capability is particularly important for use in lithium batteries which, for energy storage, have the advantages of high energy density, low maintenance, long life, light weight, and design flexibility. For hydrogen, nanotubes show promise of safe, lightweight, high-density storage, which may prove to be particularly valuable for the future hydrogen economy—in which abundant, benign hydrogen, along with hydrogen fuel cells, will supply energy for heating, cooling, electricity, industrial processes, and transportation. Carbon nanotubes and related carbon-based materials are among our best bets for meeting the DOE goal to develop systems that will store enough hydrogen for our cars and trucks to be driven more than 300 miles between fill-ups without affecting cargo or passenger space. (For more on hydrogen storage with SWNTs, see the article “New Horizons for Hydrogen” in the *National Renewable Energy Laboratory 2003 Research Review*.)

**Quantum Dots.** Quantum dots are small semiconductor nanocrystals with diameters that range from about 2 to 10 nm and that typically contain from hundreds to thousands of atoms. Because of their small size, quantization effects become important. Quantum dots confine electrons to discrete, widely separated energy levels, which gives the dots optical and electronic properties that are dependent on the size of the dots and the material out of which they are made (see sidebar “Quantum Confinement: Shifting toward the Blue”). This makes them particularly valuable for solar cells, as a pathway toward high efficiency and low cost.

NREL makes several types of QDs, including CdSe, CdS, CdTe, InP, InAs, PbSe, and PbS. We

### Quantum Confinement: Shifting toward the Blue

A salient feature of QDs is that they can be tailored to absorb or emit specific wavelengths of light simply by changing the size of the dot. Compared with the bulk material, the light spectra emitted or absorbed by QDs will shift to the blue (greater energy or shorter wavelength); the smaller the dot, the greater the shift. The shift is dependent on the size of the dot and the type of material.

Why does such quantized absorption or emission happen? Fundamental to quantum physics is the concept of the wave/particle duality of matter. For example, an electron can be thought of either as a particle or as a wave moving through its space. In bulk material, electrons exist at many energy levels—in fact, a continuum of energy levels in

valence and conduction bands—because of the numerous atoms in the material. (No electron, however, can exist in the forbidden region between the top of the valence band and the bottom of the conduction band.) But, as the size of a material approaches the nanoscale, it starts to confine the energy levels at which an electron may exist.

To see why, think of an electron as a wave and the QD as a sphere with a diameter approximately the size of the Bohr radius, which confines the electron (see also sidebar “Excitons”). In such a confinement, the electron has to travel within the inside circumference of the sphere so that its wavelength does not destructively interfere with itself. This means that the confining circumference must be equal to the electron wavelength or some whole number multiple of



make dots in two ways (both of which can be self-organizing): epitaxial growth and colloidal chemistry. Epitaxial growth is the growth of crystals of one semiconductor material on the surface of another, in which both materials have the same structural (lattice) orientation. NREL researchers are exploring a particular version of epitaxial growth known as Stranski-Krastanow growth, in which a mismatch of the lattices produces strains between the two materials causing islands to form. Most of the deposited material will accumulate on the islands, thus forming a matrix of QDs, whose size can be directed by controlling the growth conditions. To make these QDs, researchers use either of two well-known vacuum technologies: molecular beam epitaxy or metalorganic chemical vapor deposition.

Colloidal chemistry, however, is NREL's primary method of making quantum dots. This is an inexpensive way to grow the dots, requiring only the right chemicals, low-cost equipment, and room-temperature processing. Colloids are ultra-fine particles suspended in a liquid solution—colloids are formed by not having the solute molecules break up into atoms and thus dissolve. The formation of QDs involves a chemical reaction between a metal ion (such as indium) with a molecule that donates a different ion (such as phosphide). The size of a QD is manipulated by controlling the concentration of the reactants, the medium in which they react, the temperature of the reaction, and the length of the reaction.

The trick is to keep QDs from agglomerating when they have reached the desired size. This is done generally by having the reaction take place in the presence of organic molecules that act as surfactants and coat the surface of the nanoparticles—the organic molecules stop the crystals from clumping together.

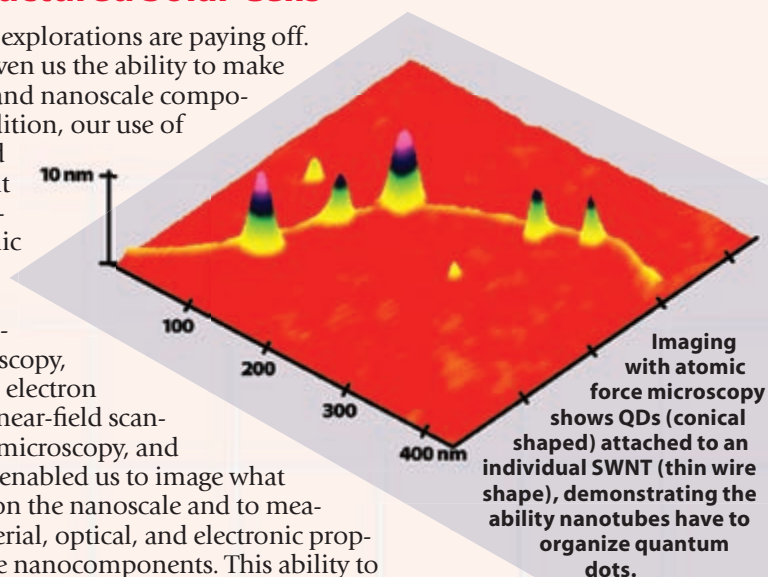
**Nanorods.** These are semiconductor rods that are typically on the order of 2–10 nm in diameter and tens to several hundreds of nanometers long. It is the small diameter that promotes quantization effects and gives them similar characteristics to quantum dots. Nanorods, however, are unconfined in one direction, and charge carriers are free

to move along the length of the rod. Nanorods of some materials can be grown using colloidal chemistry in a similar manner to QDs, except that growth is promoted along one axis and retarded along the other two axes via appropriate control of the growth solution, growth kinetics, and surfactants. There are other methods being explored to grow nanorods, such as via nucleation in a super-saturated solution. Nanorods of particular interest to NREL include CdS, InP, PbSe, PbS and several oxides, such as ZnO and TiO<sub>2</sub>. Like QDs, nanorods are particularly promising for use in solar cells (also see sidebar “Printing Polymer Solar Cells”).

## Nanostructured Solar Cells

NREL's early explorations are paying off. They have given us the ability to make and understand nanoscale components. In addition, our use of sophisticated measurement techniques—such as atomic force microscopy, scanning tunneling microscopy, transmission electron microscopy, near-field scanning optical microscopy, and more—have enabled us to image what is occurring on the nanoscale and to measure the material, optical, and electronic properties of these nanocomponents. This ability to make, measure, image, and model nanoscale components and systems has given us the tools with which to proceed to the next important step—to build composite devices and systems with new properties that will allow us to do new things.

Among these new composite systems is nanostructured solar cells. Solar PV cells represent an extremely promising technology for supplying large amounts of non-carbon energy in the future. However, to meet that promise—to be used on the massive scales needed—PV electricity has to be competitive with the least-costly alternative. This means the present cost of PV electricity has to be decreased by at least three- to fivefold to 6¢/kWh, or less. Plus, if PV electricity is to be used to competitively produce hydrogen (via the electrolysis of water) on a central-station scale for the future hydrogen economy, the cost has to be reduced by at least another factor of two to three.



the wavelength. If it is other than this, the wavelength would interfere with itself and destroy its possibility of existing.

Thus, only certain (quantized) wavelengths can exist in such a confinement. The shorter the diameter of the confinement, the shorter the wavelength of the electron. And because energy is inversely proportional to wavelength (directly proportional to frequency), the smaller the QD, the smaller the allowable wavelength, the greater the frequency, and the bluer the associated photon emission or absorption spectra.

The same phenomenon holds for nanorods. But in this case the rod is to be likened to a cylinder and the confinement space dictated by the diameter of the cylinder.



Today, PV electricity costs about 18–30¢/kWh, depending on the application and its scale. The technology that has dominated the PV market for the past two or three decades—the so-called *first-generation PV technology*—is based on thick (150–300  $\mu\text{m}$ ) cells of crystalline silicon. Although a mature technology, further innovations and economies of scale may be able to cut the cost of silicon PV electricity by another factor of two or so.

Emerging PV systems based on thin-film layers (1–2  $\mu\text{m}$ ) of semiconductor materials—known as the *second-generation PV technology*—are currently competitive with crystalline silicon. Even though modules from these materials are not generally as efficient as those of crystalline silicon, because of the thinness of the material and the ability to use mass production, thin-film PV has the potential to drop PV costs to the aforementioned 6¢/kWh.

Even if thin-film PV meets its long-term potential, according to a report by the Basic Energy Sciences Advisory Committee we would still have to drop costs another three to six times to make it economically attractive enough to provide the scale of applications the world will need. But to achieve such cost reductions we need a quantum leap to a *third-generation PV technology*. This is where nanotechnology comes into the picture. By using nanotechnology, polymer technology, and innovative production techniques, there are two paths whereby nanostructured solar cells can reduce costs sufficiently: by making the solar cells extremely inexpensive, and by making them very efficient at converting sunlight to electricity.

## An Inexpensive Route—the Dye-Sensitized Solar Cell

Titanium dioxide ( $\text{TiO}_2$ ) is an inexpensive material that exhibits semiconductor properties. But as a solar cell material, it has a major drawback—its band gap is greater than 3 eV. The solar spectrum, on the other hand, is comprised of photons with energies ranging from 0.3 eV to 3.5 eV. So  $\text{TiO}_2$  by itself can absorb and convert only that small portion of the solar spectrum whose photons have an energy equal to or greater than 3 eV. However, scientists from NREL and elsewhere who have worked on this concept have long recognized that  $\text{TiO}_2$  has the potential to produce inexpensive electricity by using it in a photoelectrochemical

### Excitons

In the typical PV cell using bulk semiconductor material, incident photons dislodge electrons from their bound state in the valence band into the conduction band. A dislodged electron leaves behind a hole of opposite charge. This electron-hole pair is bound together by the coulomb force as a neutral excited state. The distance between the electron and the hole is known as the Bohr radius and is typically on the order of a few nanometers.

In bulk PV semiconductors, the freed electrons and holes can move freely in all directions. And because there are an immense number of atoms connected via crystalline lattice networks, the coulomb attraction between an electron and its hole can be weakened because of screening by other atoms and the lattice, and because of the mass of the constituents of the material. As a result of this weak coupling, electron-hole pairs readily dissociate at room temperature and can be swept to opposite sides of the PV cell

cell with an appropriate dye that can absorb much of the solar spectrum.

The basic design of the cell consists of  $\text{TiO}_2$ , the dye, and electrolyte sandwiched between a transparent conducting oxide (TCO) electrode and a counter-electrode (see figure). The sunlight excites and oxidizes the dye molecules, which produce electrons that are injected into the conduction band of the titanium dioxide. Charge separation occurs at the interface between the dye molecules and the titanium dioxide. The electrons are transmitted by the  $\text{TiO}_2$  to the electrode to provide current for a circuit to do work and return to the cell via the counter-electrode. The oxidized dye molecules are reduced by electrons transferred by redox (oxidation-reduction) couples in the electrolyte.

This concept did not work well until used with  $\text{TiO}_2$  nanocrystals of approximately 30 nm diameter. Although these nanocrystals do not exhibit quantization effects, their use greatly increases the contact area between the dye, the  $\text{TiO}_2$ , and the electrolyte to enhance the efficiency of electron injection from the dye.

One drawback to the concept is that it uses a liquid electrolyte. But this can be circumvented by using a polymer-based electrolyte or a hole-transporting polymer; either alternative leads to longer life and lower cost and provides the ability to make flexible solar cells.

Other alternatives being explored include the use of QDs in place of the dye, or even turning to a different approach altogether—such as a polymer/metal oxide configuration (see the sidebar “Printing Polymer Solar Cells”)—to achieve a low-cost solar cell.

Although this approach has not resulted in high-efficiency solar cells—with the best dye-sensitized cells exhibiting efficiencies around 11% and modules having typical efficiencies of about 5%—it has a high potential for low cost because of the low cost of the  $\text{TiO}_2$ , the dye or the QD alternative, and the polymers and because of inexpensive



by an induced electric field (typically via doping semiconductor layers with extra electrons or holes) to be collected by a transparent conducting oxide layer or a metallic grid. Alternatively, electrons and holes could typically recombine within a few microseconds before they have a chance to be further separated for collection.

In QDs (or nanorods or conjugated polymers), the situation is different. The electron and its associated hole are close together, are not screened from each other, and the coulomb attraction between the two is quite strong (especially in conjugated polymers)—a situation that leads many in the field to label such an electron-hole pair as an “exciton.” Under such conditions, the electron-hole pairs in excitons can quickly recombine—typically on a sub-nanosecond time scale. Moreover, excitons retain a neutral charge, so you cannot use an electric field to dissociate them. Rather, excitons in QDs (and conjugated polymers) are dissociated

at interfaces with other materials that have high affinities for electrons or holes, with electrons taken in one direction at the interface and holes in another. Movement of excitons is initiated via diffusion; but with a high concentration of excitons and interfaces, this diffusion readily results in dissociation. The dissociation, in turn, sets up a chemical potential gradient that drives the PV effect.

So what can you use to scavenge the excitons and dissociate the charge carriers to produce the chemical gradient and a photocurrent? Both fullerenes ( $C_{60}$ ) and single-wall carbon nanotubes have high electron affinities that can overcome an exciton's binding energy to siphon freed electrons. Conjugated polymers, in which polymer matrices can be a combination of hole-conducting and electron-conducting can also be used to dissociate and conduct electrons in one direction and holes in another.

processing techniques available for making the cell.

This is also a versatile approach because it will enable us to explore a variety of different substrates on which the cell can be deposited, it could allow production of flexible solar cells that could fit on any surface, and it would allow other layers, such as  $WO_3$ , to be added to the device, which would merge the solar-cell function with an electrochromic function. Such a device employing other layers could be used for windows, for example, that would not only generate electricity but would also lighten or darken as desired in accordance with the amount of sunshine.

## The Road to High Efficiency

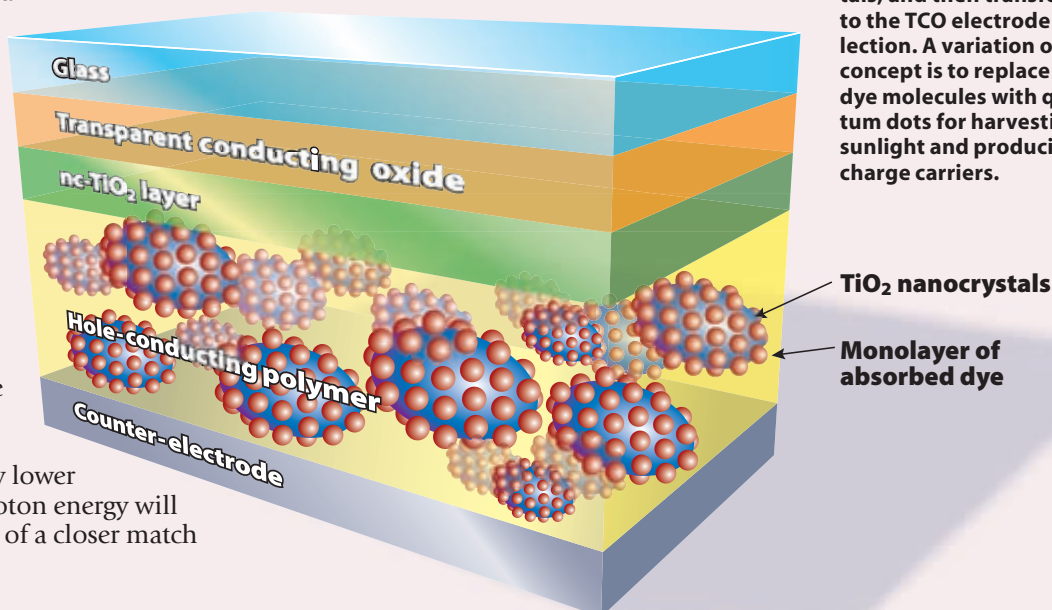
Today's typical solar cell relies on a semiconductor material with a single junction and a single band gap. Such a cell has limited efficiency because photons with less energy than the band gap will not be absorbed, while photons with energy greater than the band gap will dislodge electrons into the conduction band, but with too much energy. The excess energy absorbed by an electron will push it into a high and unstable energy level. The electron will quickly relax to a more stable level, emitting the excess energy as heat. This not only wastes the excess photon energy, but the heat it produces further decreases the efficiency of the cell.

One strategy to overcome this limitation is to use several layers of semiconductor materials with different energy band gaps, stacking the layers in decreasing band-gap order. That way, the higher energy photons of the solar spectrum will be absorbed by the higher band gap material and lower energy photons by lower band gap material. Thus, the photon energy will be used more efficiently because of a closer match

with the energy band gaps of the absorbing materials, and not so much heat will be produced. By stacking an increasingly large number of materials with different band gaps, as the number of layers approaches infinity you can approach the theoretical efficiency limits of 68% under one sun and 86% under concentration. The problem is that the engineering and physical challenges become increasingly difficult the more layers that are stacked in this manner; and costs rise accordingly. Thus far, the best cell using this approach has been an expensive three-junction device of high-quality material that attained 37.3% efficiency under high solar concentration.

Quantum dots potentially offer a way around this conundrum. Quantum dots can easily be made with different band gaps simply by controlling the size of the dots. By using different-size dots, a many-junction device can be devised to capture and convert the entire solar spectrum. By using a sufficient number of dots with differing sizes, the theoretical limits of efficiency may be approached. And it may be done inexpensively because of the use of colloidal chemistry to produce the QDs and a low-cost matrix in which to imbue them.

**The dye-sensitized solar cell represents a pathway toward low-cost solar electricity. It uses dye molecules to absorb a large portion of the solar spectrum and produce electrons, which are injected into the conduction band of the  $TiO_2$  nanocrystals, and then transferred to the TCO electrode for collection. A variation on this concept is to replace the dye molecules with quantum dots for harvesting the sunlight and producing the charge carriers.**





## Other Uses for NREL Nanotechnology...

There are many other possible uses inherent in NREL's nanotechnology research.

- **Nanocatalysis.** Catalytic reactions occur on catalyst surfaces. Because smaller particles increase surface area, nanocatalysts have the potential for a great amount of surface area to perform catalytic reactions. Other nanostructures (such as nanofibers) can also provide a large active surface area for catalyst support. The modification of electronic and material properties at the nanoscale may also play a beneficial role in catalysis. Nanocatalysis has particular promise for the production of fuels from biomass, producing hydrogen from biogas during the water-gas-shift reaction, and for use with membrane technology for the separation of hydrogen gas.

- **Gas-Separation Membranes.** Gas-separation membranes are used to separate types of gases from one another. This can be accomplished because of the porosity of the membrane materials or because of their ion- or electron-affinity. In either case, nanomaterials, especially those of carbon nanotubes, which have high electron affinity, may offer advantages. Also, because nanostructures offer advantages for catalysis, they can be used to help drive the process of gas separation. Gas separation membranes could find applications in the separation of hydrogen from biogas and in fuel-cell membranes to separate hydrogen protons from the electrons of a hydrogen atom.

## The Right Medium/ The Right Configuration

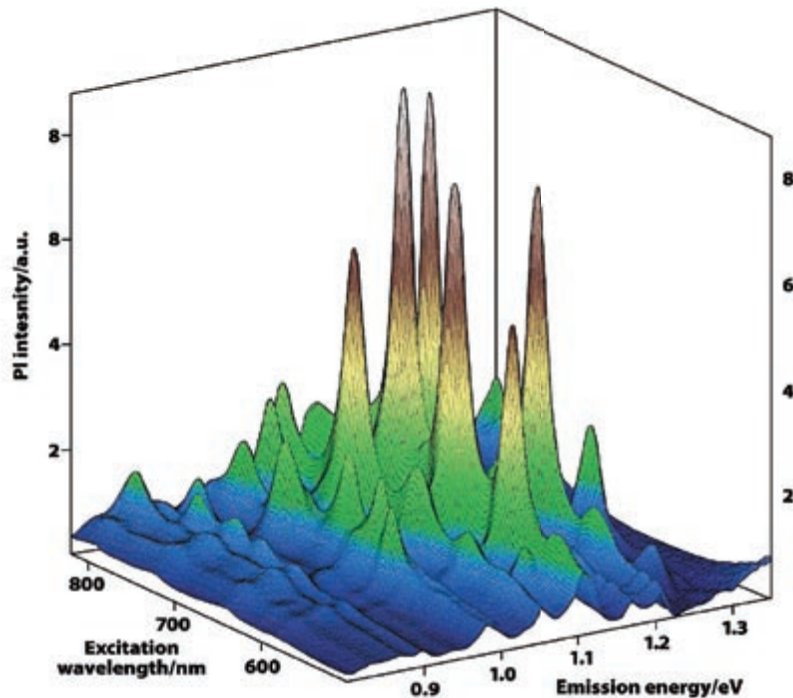
With QDs, there are immediate barriers to overcome. The first is to dissociate an exciton's freed electron from its paired hole before they recombine. This is done at interfaces with other materials, which will siphon the charge carrier, taking the hole in one direction and the electron in the other to separate grids or collection points (see the sidebar "Excitons").

One way to do this is to deposit the QDs into a medium consisting of a mixture of conjugated polymers (polymers that exhibit semiconductor properties), one of which attracts and conducts holes and the other of which attracts and conducts electrons. This is a highly desired approach because it has the potential to be a very inexpensive alternative, using plastics and colloidal QDs, and it may even allow for high efficiency.

Thus far, however, cell conversion efficiencies using this approach have generally been less than 3%–4%. Difficulties arise with conjugated polymers because they contain many sites that engender the recombination of electrons and holes; the electrons and holes of the induced excitons are strongly attracted to each other and so will quickly recombine; and the charge carriers do not have great mobility and are not quickly dissociated from one another, which increases the probability of recombination. Moreover, the conjugated polymer matrix would have to be blended correctly to ensure that most QDs were in contact with both hole- and electron-conducting polymers, to ensure a high level of exciton dissociation and conduction of charge carriers.

## Connecting the Dots

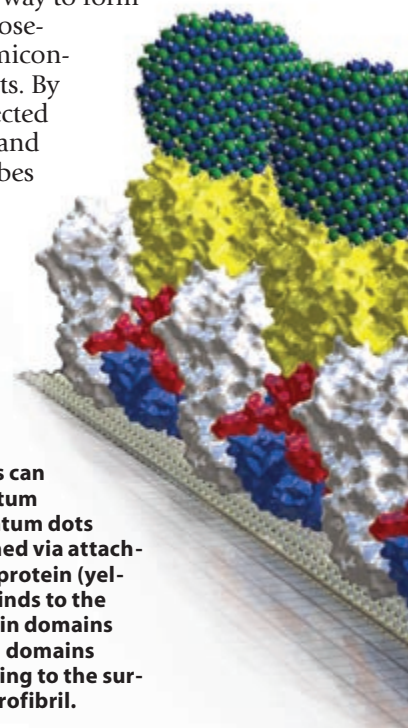
To achieve high-efficiency cells, therefore, it is better not to mix QDs randomly in a polymer blend, but to align the dots in arrays so that they communicate with one another efficiently. This could be done by arraying the dots within a few angstroms of one another to enable electronic coupling among the dots so that electrons can be transported long distances. How you align the dots into arrays becomes the hot question. NREL researchers are exploring a couple of innovative ways to accomplish this: carbon nanotubes and proteins.



In solution, SWNTs exhibit a photoluminescence spectra whose characteristics differ in accordance with the diameter of the nanotubes and their chirality. Photoluminescence occurs because of the recombination of electrons and holes induced by incident light. Such a spectra is indicative that SWNTs can be used to harvest light to generate electricity.

**Carbon Nanotubes.** The use of carbon nanotubes for organizing and connecting QDs combines the depth of experience that NREL researchers have with QDs with their expertise with single-wall carbon nanotubes. In this vein of research, scientists are exploring both chemical and physical methods to bring SWNTs and QDs into intimate electronic contact.

With one alternative, NREL researchers have developed a simple way to form one-dimensional close-packed arrays of semiconductor quantum dots. By combining size-selected InP and CdSe QDs and highly pure nanotubes



Cellulosome polymers can be used to align quantum dots. Here, CdSe quantum dots (blue-green) are aligned via attachment to a streptactin protein (yellow), which, in turn, binds to the cellulosome via cohesin domains (red). Surface binding domains (blue) are shown binding to the surface of a cellulose microfibril.



that have low defect densities, while gently refluxing both in organic solvents, linear arrays of QDs are self-assembled by van der Waals forces into the grooves between adjacent nanotubes.

In another alternative, SWNTs can be diced into short segments and solubilized in solution using surfactants, much in the same way that semiconductor colloids are typically solubilized. Once in solution, the soluble SWNTs can be treated as reagents and reacted with QDs in solution, to promote coupling among the quantum dots

One interesting characteristic of SWNTs is that they exhibit emission and absorption spectra similar to those shown by QDs of different sizes. In particular, the photoluminescence intensity of the peaks in the spectra is dependent on the diameter of the nanotubes and their chirality (i.e., their helical pitch, or how the graphite sheets roll up). This presents quite a flexibility when using SWNTs with quantum dots. Depending on the type of SWNT used to provide the coupling, the interconnection can either provide simple electronic communication among the dots (when the SWNT is a wire), or it can be used to help harvest the solar spectrum when the SWNT is semiconducting and photoactive. Here, a long-term goal is the construction of hybrid nanoscale systems in which sunlight can be efficiently harvested and converted to generate electricity or fuels, such as hydrogen.

**Proteins.** The use of proteins to align dots is a method unique to NREL researchers. To be more specific, researchers genetically modify a cellulosome protein polymer so that it will attach to quantum dots. A cellulosome is an intricate multi-enzyme complex that efficiently degrades cellulose, which is the most abundant

organic polymer on the planet. Through the Laboratory's work with biofuels, in which alcohol fuels are derived from biomass cellulose, NREL biochemists have plenty of experience with cellulosomes. Now they are working with NREL physicists to use cellulosomes to align quantum dots.

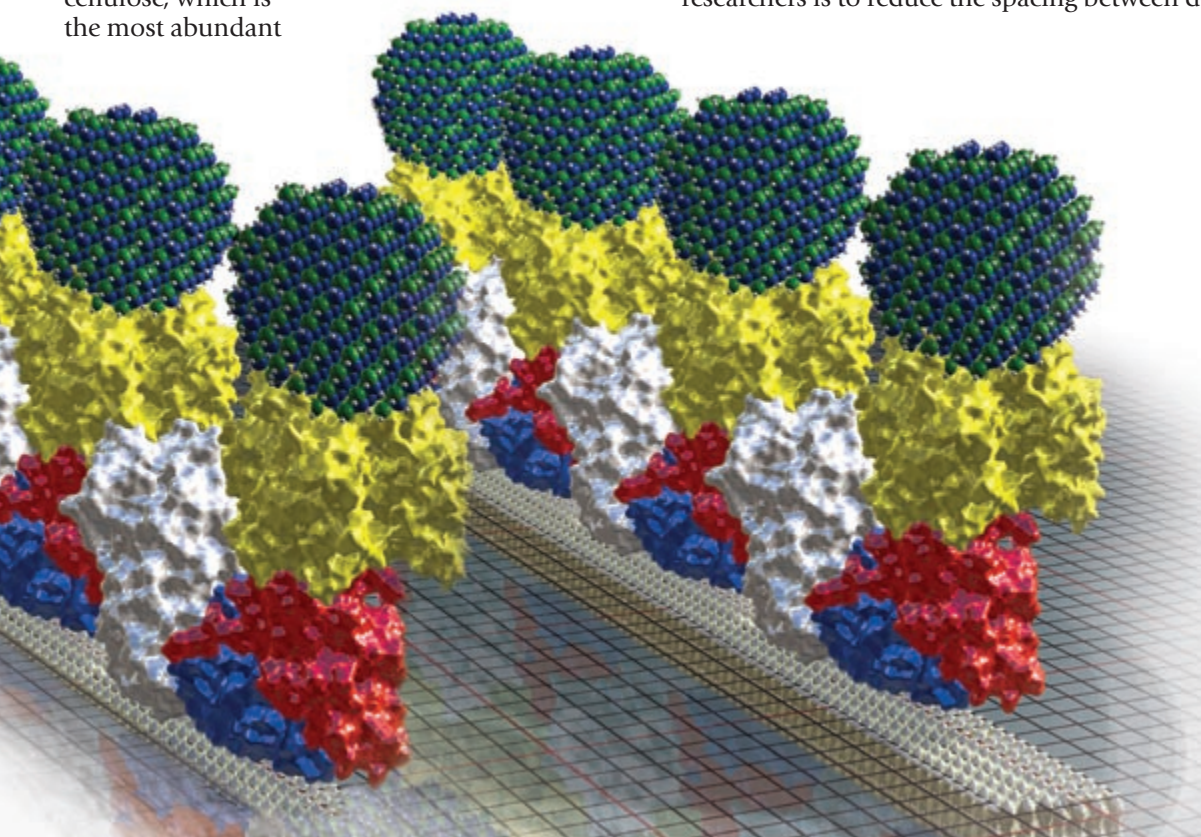
A cellulosome is a conglomerate of functional subunits. The backbone of this conglomerate is known as the scaffoldin, which organizes and integrates the subunits into a multi-enzyme complex (see figure). The scaffoldin unit contains a site known as the surface-binding domain, which enables the cellulosome to bind to a cellulose substrate. It also holds a series of cohesin domains, to which enzymes will bind via sites on the enzymes known as dockerin domains.

This is the normal order of things. But the size of the cohesin domains where the enzymes normally dock is approximately equal to the size of quantum dots. The trick, therefore, is to remove the enzymes and encourage the cohesin to instead bind to quantum dots or, alternatively, to bind to another protein, which then could bind to quantum dots. Once this is done, and because these units can self-organize into long polymer chains, this approach can be used to produce a chain of quantum dots. Consequently, using an appropriate substrate to which scaffoldin units can adhere, QDs can be maneuvered into arrays with close enough spacing to promote electronic coupling among the dots.

This is breakthrough, state-of-the-art research. Nonetheless, NREL scientists have shown it can be done using a genetically modified cohesin/dockerin polymer to align (CdSe)/ZnS QDs on cellulose fibrils. The next challenge for the researchers is to reduce the spacing between dots

## ...Even More Uses

- **Filtration of Microbial Pathogens.** NREL has developed an R&D 100-winning technology based on nanoscale ceramic fibers. Because of an extremely high surface area and a chemical affinity, these fibers are particularly useful for filtering microbial pathogens and viruses from water and for purifying blood. The fibers are also useful for eliminating heavy metals from water, biosynthesis and bone growth, catalyst support, and filtration of other liquids and gases.
- **Air Filtration.** Nanomaterials can be used in combination with desiccant materials for conditioning and dehumidifying air. In the process, nanomaterials enhance the absorption of a wide variety of particles from the air, including pathogenic bacterial and fungal spores.
- **Ultracapacitors.** Like batteries, ultracapacitors store electricity. But they do not do it chemically; they do it physically by separating positive and negative charges. Compared with batteries, they can store large amounts of electricity in a very small volume, and can deliver orders of magnitude more charge and discharge cycles. Nanomaterials, in particular carbon nanotubes, can be used in the development of ultracapacitors that will have important uses for all walks of life—from communication to transportation.
- **QD OLEDs.** Organic light-emitting diodes (OLEDs) have the great promise of emitting tunable wavelengths of light inexpensively and with great energy efficiency. Quantum dots are particularly suitable for use with OLEDs because they can be easily tuned to emit the desired wavelengths, which can be combined to yield white light.





from a minimum of 50 Å to about 30–40 Å and to make the spacing more homogeneous.

## Hot Carrier Solar Cells

But other breakthrough results may be required to approach the high-efficiency limits of solar cells. One possibility is to develop so-called “hot electron” solar cells. When a freed electron is bumped high into the conduction band by a too-energetic photon, its electronic temperature becomes quite hot (as high as 3,000 K). The hot electron will relax to the bottom of the conduction band, typically within a few hundred femtoseconds, imparting heat to the lattice as it does so.

This can be avoided by removing the hot electron for use in a circuit before it relaxes. Doing so will achieve two things: 1) use of the high-energy electron will increase the photovoltage of the device as well as its efficiency; and 2) the excess energy

will be prevented from heating the device and from lowering its efficiency.

The key to removing the hot electron is to retard its relaxation. And the key to this is to confine the exciton to a quantum dot. A hot electron will cool quickly, especially in the presence of a hole. Remove the hole promptly and, due to quantization effects of a QD, the energy levels to which the electron can readily relax will be limited. The hole can be siphoned in a matter of a few femtoseconds by imbedding the QD in the right material, and perhaps even the right polymer material. This could extend the hot electron relaxation time by one or two orders of magnitude. Combine this with a properly ordered array of QDs, and the hot electrons could be transported along the array via resonant tunneling.

Another way to utilize hot or highly excited electron-hole pairs (excitons) in QDs is to use the

## Printing Polymer Solar Cells

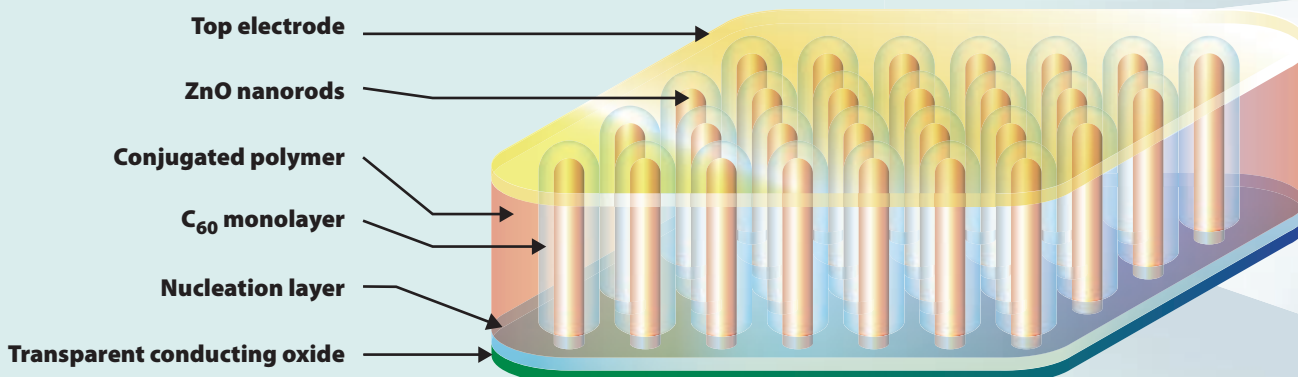
NREL scientists are combining the use of nano-, polymer, and low-cost deposition technologies in an approach that promises inexpensive solar cells. The cell concept is innovative. It starts with an inexpensive substrate on top of which is layered a transparent conducting oxide (TCO) that lets light through to the cell and acts as a cell electrode. This TCO layer can be made with nanoparticle precursors to allow constituent materials to be incorporated into an ink that can be written onto the substrate via piezoelectric inkjet printing.

A nucleation layer is then deposited on the TCO. This layer is chemically prepared to enable nanorods to grow vertically (via nucleation in a supersaturated solution) and at close intervals from the surface. The nanorods, which can be of ZnO or other oxides, grow a few nanometers thick and 200 or more nanometers long. This gives the rods a high aspect ratio (i.e., ratio of the rod's length to its width), which, in turn, promotes a great amount of surface area per given mass of material—up to 600 m<sup>2</sup>/gm. This gives the nanorods a great ability to scavenge and transport freed electrons from the surrounding material.

Next, the nanorods are coated with a thin layer (less than 20 nm) of conjugated polymer, which absorbs photons to produce excitons. Finally, a silver electrode is deposited on the polymer layer.

Although this is a state-of-the-art concept, NREL researchers have not only successfully fabricated such a device, they are already exploring ways to improve it. One way is to coat the nanorods with a monolayer of a material that has high electron affinity, such as fullerenes (C<sub>60</sub>), before the conjugated polymer is applied. In conjugated polymers, photon-induced excitons have low mobility and the electron and hole can typically recombine on a sub-nanosecond time scale. That is why C<sub>60</sub> (or some other material with high electron affinity) would be valuable in such a device; it could quickly dissociate excitons and extract electrons from the polymer and transfer them to the ZnO nanorods, which would conduct the electrons to the TCO. This would enable the conjugated polymer to conduct the dissociated holes to the silver contacts.

The device can be designed so that excitons will travel only 5–20 nm before encountering an interface. This





excess energy to create multiple electron-hole pairs. NREL researchers have found that up to three excitons per photon can be created in small band gap semiconductor QDs when the photon energy is four times the QD band gap. This approach is very promising for creating much more efficient nanocrystalline solar cells.

The exploitation of hot electrons is just one of the cutting-edge nanotechnology concepts being explored by NREL researchers. But breakthroughs in this area, along with continued advances in QDs, nanorods, carbon nanotubes, conjugated polymers, and other related fields discussed here have the potential not only to present the world with inexpensive renewable electricity, but also to provide it with plentiful non-carbon energy in all usable forms—for transportation; building heating, cooling, and lighting; and industrial processing needs.

enhances the ability of electrons and holes to be separated more quickly than they may recombine. By designing a device in which electrons and holes are separated at interfaces in a few tens of femtoseconds ( $10^{-15}$  seconds) or less, charge carriers are efficiently collected to produce an electric current.

Such a concept has great potential. Researchers believe, for example, that there may be the possibility that much of the device—the TCO, the fullerenes, the polymer, and the silver electrode—could be deposited via inkjet printing. Also, because conjugated polymers may be chemically altered to exhibit different absorption characteristics, there is the potential that they could be tuned to absorb the entire solar spectrum to produce carriers. One way of doing this is to chemically tune the band gap by modifying the conjugated polymer backbone. Another way is to attach side chemical groups to the polymer backbone.

Effectively, each nanorod/C<sub>60</sub>/polymer combination can be considered a minicell, connected to the silver electrode on one end and to the TCO electrode on the other. This opens the door for tuning each minicell

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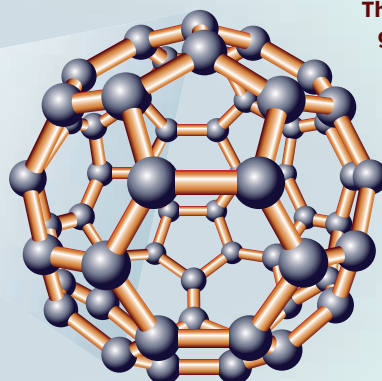
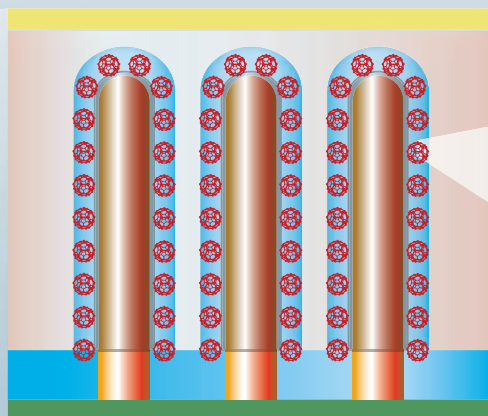
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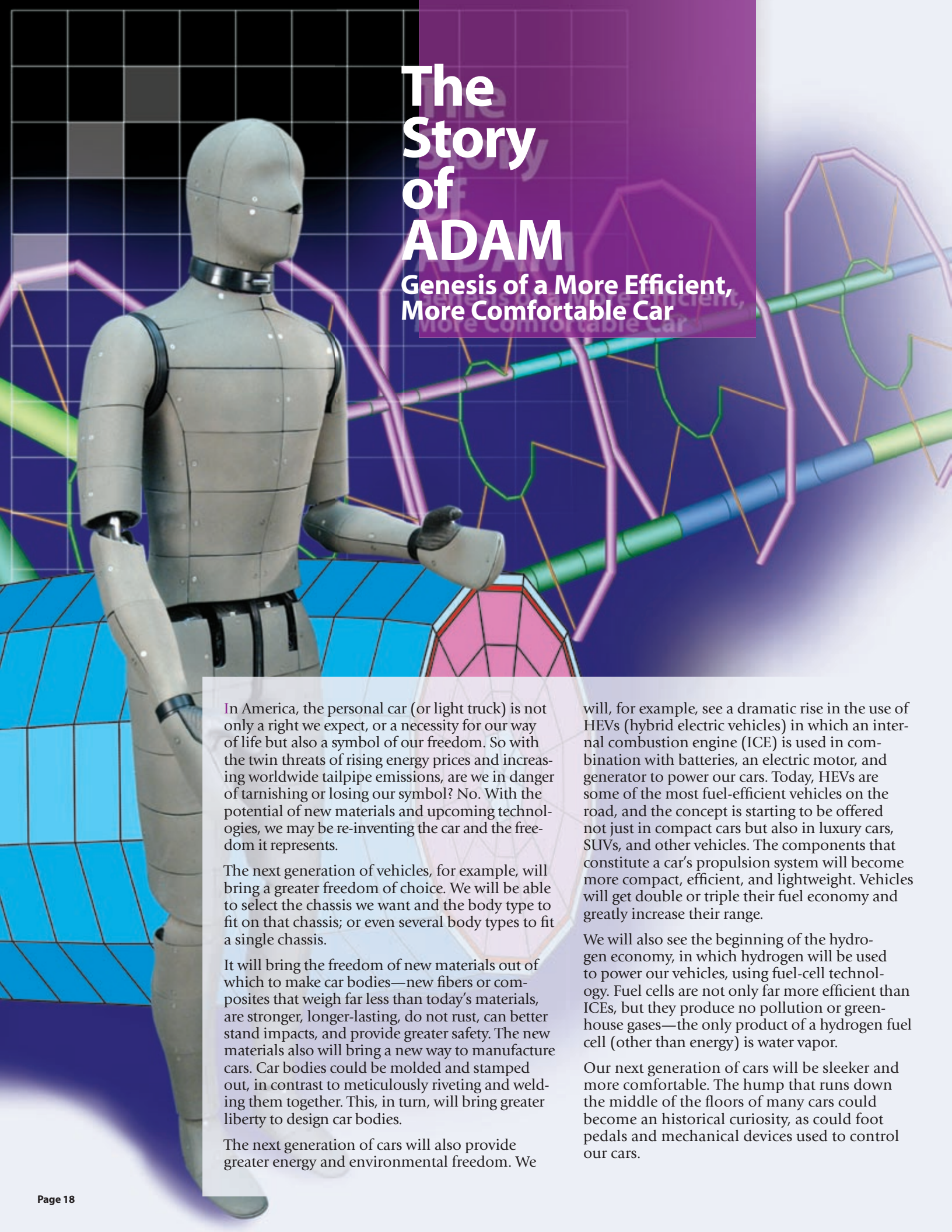
combination to different wavelengths of light. Thus, a cell like this could become a many-junction device that could efficiently absorb and convert the entire solar spectrum to excitons.

Such a solar cell would have many advantages. The entire cell, for example, would be approximately 200 nm thick and would thus use very little material. It could be made on an inexpensive and flexible substrate to fit surfaces as needed. There is the possibility that almost the entire structure could be made using solution chemistry, nanoprecursor inks, and inkjet printing. The entire device could be processed at temperatures below 400°C, and probably at less than 200°C—both of which are far lower than the temperatures at which solar cell are currently processed. The device could be made without using vacuum technology, using much less expensive equipment. And it could be made translucent, for use on such spaces as windows to allow lighting and to produce electricity. All of this could add up to the potential for an extremely inexpensive solar cell and affordable electricity.



This solar cell concept uses conjugated polymer to harvest light and produce excitons, C<sub>60</sub> to dissociate electrons from the excitons, ZnO nanorods to transport the electrons to the TCO electrode, and hole-conducting polymer to carry holes to the silver electrode. With the potential for tuning the cell to absorb and convert much of the solar spectrum and to inkjet print much of the cell, this approach could result in very inexpensive electricity.





# The Story of ADAM

Genesis of a More Efficient,  
More Comfortable Car

In America, the personal car (or light truck) is not only a right we expect, or a necessity for our way of life but also a symbol of our freedom. So with the twin threats of rising energy prices and increasing worldwide tailpipe emissions, are we in danger of tarnishing or losing our symbol? No. With the potential of new materials and upcoming technologies, we may be re-inventing the car and the freedom it represents.

The next generation of vehicles, for example, will bring a greater freedom of choice. We will be able to select the chassis we want and the body type to fit on that chassis; or even several body types to fit a single chassis.

It will bring the freedom of new materials out of which to make car bodies—new fibers or composites that weigh far less than today's materials, are stronger, longer-lasting, do not rust, can better stand impacts, and provide greater safety. The new materials also will bring a new way to manufacture cars. Car bodies could be molded and stamped out, in contrast to meticulously riveting and welding them together. This, in turn, will bring greater liberty to design car bodies.

The next generation of cars will also provide greater energy and environmental freedom. We

will, for example, see a dramatic rise in the use of HEVs (hybrid electric vehicles) in which an internal combustion engine (ICE) is used in combination with batteries, an electric motor, and generator to power our cars. Today, HEVs are some of the most fuel-efficient vehicles on the road, and the concept is starting to be offered not just in compact cars but also in luxury cars, SUVs, and other vehicles. The components that constitute a car's propulsion system will become more compact, efficient, and lightweight. Vehicles will get double or triple their fuel economy and greatly increase their range.

We will also see the beginning of the hydrogen economy, in which hydrogen will be used to power our vehicles, using fuel-cell technology. Fuel cells are not only far more efficient than ICEs, but they produce no pollution or greenhouse gases—the only product of a hydrogen fuel cell (other than energy) is water vapor.

Our next generation of cars will be sleeker and more comfortable. The hump that runs down the middle of the floors of many cars could become an historical curiosity, as could foot pedals and mechanical devices used to control our cars.



And they will have A/C (air conditioning) components, systems, and strategies that will make you more comfortable on a hot day and do it more efficiently, saving considerable energy.

## ADAM—Helping to Design Efficient Ancillary Systems

This is where ADAM (NREL's ADvanced Automotive Manikin) comes in, to help us design systems and strategies to make you more comfortable in your car. ADAM may be a manikin, but he's more than a crash-test dummy.

Crash-test dummies are made of materials to simulate humans during crash tests. They have sensors in the head, neck, legs, torso, and feet that collect and relay information about results of the crash tests—acceleration and deceleration, forces on different parts of the body, and the deflection of parts of the body during a crash. This information has helped auto makers design and build cars that are far safer than those of decades ago. Today, you would be hard put to find a new car without seat belts, air bags, a collapsible steering column, and more, all as standard features.

ADAM is analogous to crash-test dummies except that he breathes, heats, sweats, and tells us how comfortable he is. But we don't crash him into walls or ram things into him. Rather, we put him into hot (or cold) cars to see how he feels and to see how we can make him comfortable. ADAM will do for efficiency and comfort what crash-test dummies did for automobile safety. The information he generates will help us design cars that will cut the energy a car uses for ancillary loads—like climate control, power steering, lighting, water and oil pumping, all of which require fuel but are not used to propel the vehicle.

When operating, the most energy-intensive of these is the A/C load. To see why, consider that your body generates 100–150 W of heat. But to cool you down, your car uses up to 6,000 W of power. This is because the A/C system is designed not simply to cool you, but also to cool the entire car for the worst-case scenario—in Phoenix, Arizona, in the height of summer after the car has been soaking in the hot sun.

Using this kind of vehicle-cooling strategy, the United States today consumes about 7 billion gallons of gasoline per year just to cool its cars. This is equivalent to nearly 10% of the oil we import, which costs the nation about \$13 billion per year. It also adds considerably to air pollution, increasing the tailpipe emissions of nitrogen oxides, carbon monoxide, and hydrocarbons.

This need not be. We can cool our cars far more efficiently, more quickly, less expensively, using far less fuel, and be more comfortable in the bargain. To accomplish this, we have to design new components and systems and test the results of incorporating them into our vehicles. But to test

a wide variety of people with different comfort zones and in different conditions would be time-consuming and expensive. This is where ADAM comes in, as a surrogate for this testing, which will help streamline the process for design and implementation.

## Three-Part Harmony

To be a reliable proxy for how we sense and respond to heat and cold and how comfortable we feel, ADAM the manikin cannot stand alone. Rather, he is simply the physical, sensing component of a three-part system that also has a regulatory component (a physiological-response model), and a feeling component (a thermal-comfort model).

**ADAM the Sensor.** As a manikin, ADAM can sense and respond to the environment, but his response is directed and controlled by the physiological response model. ADAM is designed to represent the 50th percentile American male. He is 5 ft. 9 in. tall (175 cm) and weighs about 136 lbs. (61 kg). He is flexible at the waist, and has adjustable pre-tensioned joints at the knees, feet, wrists, elbows, and shoulders that allow him to be posed in various positions, most notably sitting behind the steering wheel of a car.

ADAM has two major layers—a skeleton and a surface layer (skin). The skeleton is made of laminated carbon fiber, making it light and strong. It supports the structure and houses internal components: energy storage in the thighs and torso; communication modules that allow the manikin to remotely communicate with the physiological model (ADAM also can be plugged into a power supply for continuous, non-remote communication); water storage, from which water is sent to the skin to enable sweating; and “lungs” that simulate breathing with exhalation of warm humid air. Through its joints, the skeleton also allows passage of wiring harnesses and sweat tubes, to enable communication with the skin.

The surface layer is composed of 126 individual segmented sections, each of which is a stand-alone unit of intricate design. Each section has several layers—an outer, low-porosity metal layer through which water is distributed for sweating; a high-porosity metal layer that distributes the water to the outer layer; and a carbon fiber structural backing, in

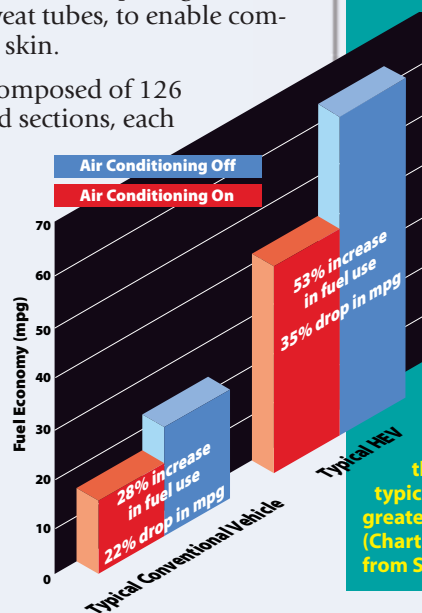
## Driving Cool in Your HEV

So you finally bought an HEV—a model that emits about one-third the greenhouse gases and is rated at 63 mpg, nearly three times the gas mileage of a typical car. It's a comfortable, sleek car with snappy acceleration. And it's so quiet that you sometimes don't know that it's on.

To take it on its inaugural spin, you get on the interstate, accelerate to an easily maintained speed of 70 mph, switch on the A/C, and cruise down the highway for 410 miles, at which point you exit the interstate to fill the gas tank. Then comes the surprise. You used 10 gallons of gasoline. That's only 41 miles per gallon! What gives?

The culprit is your A/C system. Your car's engine powers the same type of 4-kW, inefficient, vapor-compression A/C system powered by the average American car. The problem is, your HEV engine is a 1-liter, 70-hp engine, whereas typical sedan engines range from 2–3.5 liters and 160–250 hp. It takes about the same power to drive the A/C systems for both cars. But that power has a relatively higher impact on the smaller engine. So your car will experience a greater drop in gas mileage than will the typical, non-HEV vehicle. (Nonetheless, your HEV will still get more than twice the mileage than will the normal car driven with the A/C system on.)

What can be done? On your part, cut back on the use of the A/C when possible. In the long run, ADAM will play a part by testing and helping optimize the design of better ancillary systems to reduce the cooling load, including the design of more efficient A/C technologies. (See the sidebar “A Sound Idea for a Cool Car.”)



Running the A/C has a relatively larger impact on a high-mileage HEV than it does on a more typical car. Still, the HEV will get greater absolute gas mileage. (Chart is based on test data taken from SC03 driving cycles.)



Outer surface: low-porosity metal

Distribution layer: high-porosity metal

Water barrier layer

Fine grid distributed heater wire

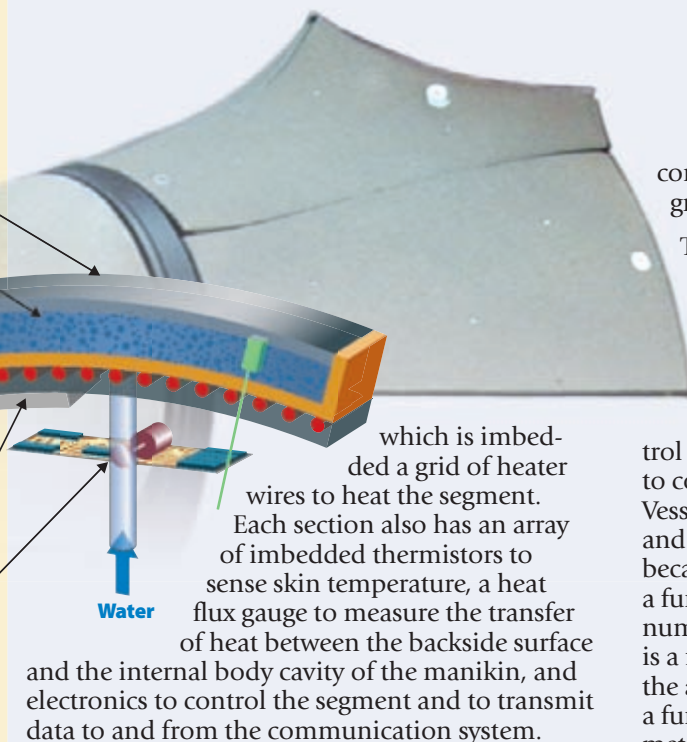
Carbon fiber structural backing and insulation

Multiple temperature sensor array

Backside heat flux gauge

Local controller and fluid control valve

A three-dimensional detail of a surface segment shows its sophisticated construction and design, which enables it to sense and respond to heat and to control sweating.



which is imbedded a grid of heater wires to heat the segment. Each section also has an array of imbedded thermistors to sense skin temperature, a heat flux gauge to measure the transfer of heat between the backside surface and the internal body cavity of the manikin, and electronics to control the segment and to transmit data to and from the communication system.

Because of this segmentation, ADAM can cool or heat different sections of his body at different rates, depending on the environmental conditions to which parts of the body are exposed.

**Central Control.** Although ADAM is a sophisticated surface sensor that measures rates of heat loss in each zone, he does not respond on his own. Instead, he sends 120 sets of data on surface heat fluxes to the computer-based physiological-response model (120 sets because 6 of the 126 surface-layer segments are controlled in pairs). Using these data, the model predicts breathing rates, local skin temperatures, and sweat rates, and transmits the set points to ADAM. Based on the set points, ADAM adjusts his heating systems and sweat and breathing rates accordingly. Then, as ADAM interacts with the environment, he transmits the resultant changes in heat flux back to the model to continue the cycle.

The physiological-response model contains a detailed simulation of human internal physiological systems and thermoregulatory responses. The model consists of a human tissue system and a thermoregulatory system. The human tissue system represents the human body, including the physiological and thermal properties of the tissues—the bone, muscle, fat, and skin in arms, legs, and torso. It also includes the lung, abdominal, and brain tissues. The model calculates

conduction heat transfer based on temperature gradients between tissue nodes.

The thermoregulatory system simulates the circulatory system and the respiratory system, the flow rates of these systems, and the heat transfer due to conduction within the fluids, mass transfer of fluid, and convective heat transfer to tissues. It also controls physiological response, such as vasomotor control (how nerves and muscles cause blood vessels to constrict or dilate), sweating, and shivering. Vessel constriction and dilation varies with skin and core temperatures and with each body zone because of vessel diameters. Sweating response is a function of skin and core temperatures and the number of sweat glands in each zone. Shivering is a function of skin and core temperatures and the amount of muscle in each zone. Blood flow is a function of skin and core temperatures and the metabolic rate.

The physiological-response model consists of about 40,000 nodes and elements. Because the model is so detailed, it presents a fairly complete picture of temperature distribution. As a result, it accurately simulates temperatures, heat transfers, and physiological responses to heat transfer. But it cannot by itself tell ADAM how comfortable he ought to feel. That part belongs to the thermal-comfort model.

**Feelin' Good.** By themselves, sensing and physiological responses have little value for designing systems to help passengers be comfortable in their cars. That responsibility falls to the thermal-comfort model. This empirical model is based on work done at the University of California at Berkeley, in which human subjects were tested in transient and steady-state thermal conditions to determine their perceptions of local and overall thermal comfort. Using this testing data, the model predicts the local sensation of 19 body parts, the comfort of those parts, the overall sensation (given the input on local sensations), and the overall comfort. Plus, the model predicts how quickly a body or parts of the body will become comfortable under transient thermal conditions.

ADAM the manikin does not directly “talk” to the thermal-comfort model. Instead, the “conversation” is between the two models. The

### A Sound Idea for a Cool Car

NREL engineers are working on an idea that could make good use of the waste heat from your car's exhaust system. They are researching a device that would use that heat to produce sound and then use the sound to cool your car—a concept known as thermoacoustic cooling.

Thermoacoustic effects have been understood for more than 100 years. However, only over the past two decades has substantial improvement been made to the design of thermoacoustic engines and refrigeration cycles. Recent thermoacoustic refrigerators have flown on the space shuttle and cooled electronics in a Navy destroyer. The idea is

simple . . . the waste heat from your vehicle can be used to set up a temperature difference across a pile of plates or “stack.” During periodic fluctuations in gas pressure, the gas passing through the stack is heated at the proper phase in the acoustic cycle to amplify the oscillations—much like light waves in an optical laser. The imperfect thermal contact in the stack's pores provides the phasing between compressions, expansions, and acoustic displacement necessary to lead the gas through the desired thermoacoustic cycle.

Furthermore, our thermoacoustic device pumps heat using standing sound waves to take the working fluid (helium) through a thermodynamic cycle. We rely on the heating and



physiological model sends sets of surface temperature data and core temperature data to the thermal comfort model, which uses that data to determine local and global sensations. It then uses the local and global sensations to determine the local and global comfort of ADAM the passenger.

## A More Comfortable Car

Given this, we are now ready to dress ADAM, put him in a car, subject him to different environmental conditions, and test ancillary systems to see how effective they are in making him comfortable, while trying to save energy at the same time. Dressing him is important because the clothes he wears affect the transient thermal response.

What kind of ancillary systems will our research help make possible in our next generation of cars because of ADAM? There are many. We can, for example, design better windshields and windows that will substantially reduce solar radiation entering the vehicle, while allowing visibility that is as good as typical windshields. Especially in hot, sunny climates, solar radiation will quickly heat a car and necessitate the use of substantial A/C energy to cool the car down. Advanced windshields and windows could also be designed with coatings that could quickly de-ice them in cold weather without having to rely on defrosters.

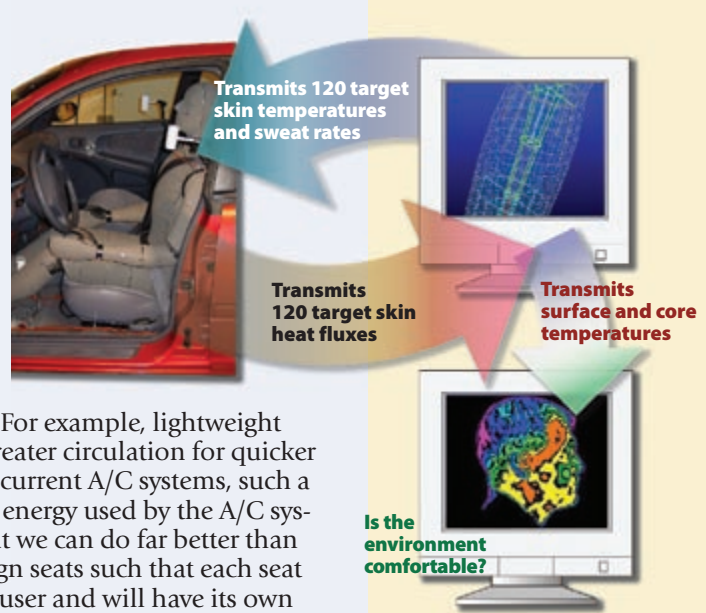
We could also design cars that are ventilated when parked, to dissipate heat when a car is left to soak in the sun. This would save A/C energy that may otherwise have to be used to cool the car from a high temperature.

A major improvement would be advanced A/C systems. Rather than rely on engine-driven vapor compression, we could use the heat from exhaust systems to cool our vehicles. There are several concepts being explored for this, including absorptive cooling (which uses an absorption refrigeration cycle rather than a vapor compression cycle), metal hydride cooling (in which the endothermic reaction—a reaction that pulls heat from the environment—of desorbing hydrogen from a metal hydride can cool the vehicle); or thermoacoustic cooling (in which waste heat is used to produce sound waves, which generate compression and expansion cycles to cool the

vehicle—see sidebar “A Sound Idea for a Cool Car”).

Something ostensibly as simple as seats can save significant energy while making you more comfortable. For example, lightweight mesh seats allow greater circulation for quicker cooling. Even with current A/C systems, such a seat can reduce the energy used by the A/C system by 3%–5%. But we can do far better than this. We could design seats such that each seat will conform to its user and will have its own individual A/C system in which low-velocity cool air circulates along your body on demand to cool you, without having to cool the entire car. Moreover, we could combine such a system with the use of new approaches in A/C systems, such as thermoacoustic cooling.

By using ADAM to test and prove such new concepts, we will be able to help the automotive industry incorporate a wide variety of advanced ancillary systems in our cars and light trucks. This could decrease our use of energy for ancillary systems by 75% or more. If we project that kind of reduction to a national level, our next generation of cars and trucks could reduce the nation’s consumption of gasoline by 5 billion gallons per year, just for our A/C systems.



**The three-part system:** 1) ADAM the manikin, which senses temperature and sends data on heat flux to the 2) physiological-response model, which predicts the local skin temperatures and sweat rates, and transmits the set points to ADAM to control sweat and breathing rates, and 3) the thermal-comfort model, which determines the comfort of the manikin and its various segments based on surface and core temperature data received from the physiological model.

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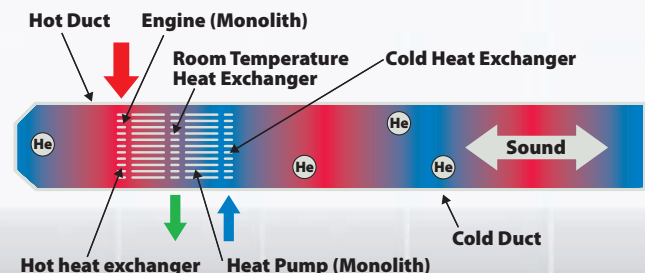
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“Thermal Comfort Project: A Cool Solution to the Nation’s Energy Security Challenges.” Center for Transportation Technologies and Systems (CTTS) Fact Sheet. (2002). 2 pp.; NREL Report No. FS-540-32285.

cooling that accompany the compression and expansion of a gas in a sound wave to produce the cooling for the interior of the vehicle.

This concept has many potential advantages over a conventional A/C system. It uses waste heat, is reliable and inexpensive, does not entail the use of an extra energy load on the engine, relies on gases that are environmentally benign, has no sliding parts (and thus should have a long lifetime), and requires no lubrication. The down side is, because of its low energy density, the device could take up a lot of volume. If we can overcome that barrier, it could be one of the cool technologies in your next-generation car.



In a thermoacoustic device, the heating and cooling that accompany the compression and expansion of a gas in a sound wave produces cooling for the interior of the vehicle.



A large offshore wind turbine is shown in the ocean. The turbine has three white blades and a yellow and white striped tower. In the background, another smaller wind turbine is visible. The sky is blue with some clouds. A white grid pattern is overlaid on the entire image.

# Harvesting the Ocean Wind

## Generating Electricity with Deep-Water Wind Turbines

Throughout history, Europeans have relied on the sea for sustenance, and once again they are turning to the oceans to harvest energy from the wind. The first to do so was Denmark when, in 1991, it placed 11 turbines off the Atlantic coast near the port of Vindeby. Since then, the concept of offshore wind energy has been gathering momentum, with 17 projects currently providing 600 MW of generating capacity off the shores of northern Europe.

For Europe, this is just the beginning. According to the European Wind Energy Association, another 150 wind projects are being planned, targets that call for an additional 70,000 MW of offshore capacity by the year 2020. In contrast, the United States does not yet have offshore wind farms, but there are some on the drawing boards.

Why the discrepancy between continents? Europeans have long enjoyed greater financial incentives for wind development. For example, Germany offers low-interest loans for wind development. Ireland forgives taxation on a portion of utility company profits reinvested in renewable energy. However, geography plays a major role as well—in much of northern Europe there is a scarcity of land-based wind sites with adequate resource. This is compelling the wind industry in nations such as Denmark, Germany, and Great Britain to move offshore where winds are stronger, steadier, and abundant.



In the United States, where the land-based wind resource in the Midwest is abundant, the incentive to go offshore is not as obvious until one compares the proximity of the major East Coast load centers with the wind resources. Projects located in the ocean can avoid long-distance electric transmission bottle necks and take advantage of the local high winds. The most publicized offshore undertaking in this country has been the Cape Wind project, proposed to stand in waters several miles from Martha's Vineyard, Massachusetts. The prospect of a wind farm has raised objections from some residents who think the turbines could ruin their view. Others back the project, including environmental groups such as Greenpeace and the Union of Concerned Scientists.

In New York, the Long Island Power Authority has proposed another offshore wind farm that could soon add 140 MW to the electric grid—a proposal that thus far appears to meet the approval of some Long Island organizations, the Governor, and several environmental groups.

Ideas that have incubated for years in the labs of NREL's National Wind Technology Center could create technologies to enable wind farms to generate electricity much farther away from the shore—in deep water, where the winds are stronger, windy sites are an order of magnitude more abundant, and land-use conflicts are easier to mitigate. With an aggressive R&D program to push it forward, researchers believe this technology could be economically feasible in 10–15 years.

How deep is deep water? "There is no universal definition," says scientist Walt Musial. "For purposes of discussion, let's say it's the depth where we would need substantial new technology." Currently that depth is 20 or perhaps 30 meters, he says. Beyond that, it is no longer practical to use the monopole construction of today's turbines, in which a steel pole 5 meters or more in diameter is driven into the seabed floor.

Floating platforms of the kind used in offshore oil and natural gas drilling may be replacing the monopole. Variations of this theme are being computer-modeled by NREL's wind scientists, working with researchers from the Massachusetts Institute of Technology (MIT). Using wind turbine codes such as FAST or ADAMS with MIT's floating structures dynamics code, SML, they strive to simulate the inevitable rocking motion of a floating platform with the workings of a wind turbine. By approximating the load environments in which offshore wind turbines operate, their work will foster more reliable turbine design tools, and better techniques for reducing the uncertainty of offshore wind turbines.

A challenge inherent to farther-out wind farms is transmitting the power to shore. From today's turbines, electricity is transferred via submarine electric cables. Greater distances will add cost, but it

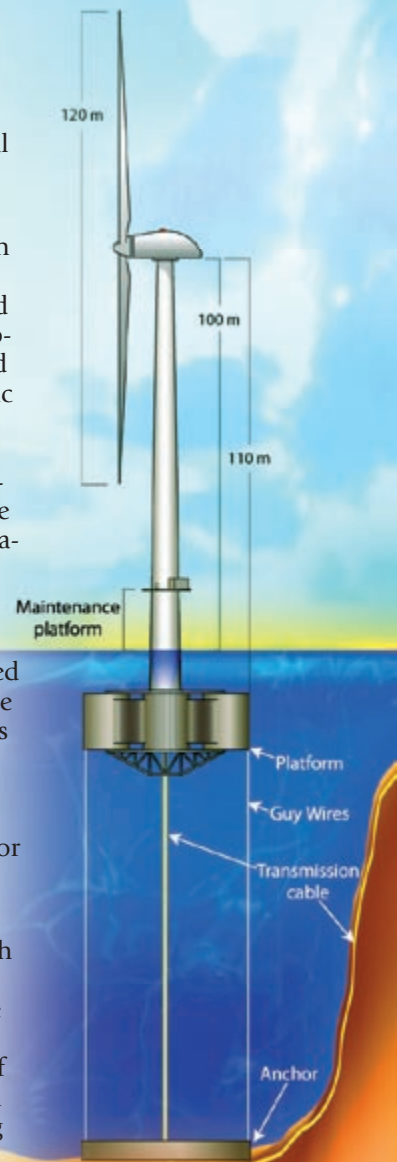
won't necessitate any radical new science, Musial believes.

One idea for transferring energy is tied to the vision of a future "hydrogen economy," in which hydrogen would be a major fuel and energy carrier for the nation. At remote wind sites (on land as well as at sea), electricity could be used to produce hydrogen from water. This approach would not only obviate the need for investing in electric cables and infrastructure, it would also provide a high-value dispatchable energy source whose production and use would emit no carbon dioxide. The hydrogen would be transported to shore and used to supply fuel and power for transportation, industry, and other applications.

Aside from technological advances, large-scale deep-water offshore wind development would require new thinking, says Musial. "We've learned a lot about the use of floating platforms from the oil and gas industry, but we couldn't do business the same way. Our intent would be to leapfrog the status quo." For example, wind developers would seek economies of scale by manufacturing platforms by the hundreds, rather than one or two at a time as in the petroleum industry.

New thinking would also evolve from management practices at today's wind installations, both offshore and land-based. Operation and maintenance costs for offshore installations might be triple those of land-based systems. Turbines off the European coasts currently experience a lot of downtime because they are often inaccessible in severe weather. NREL researchers are developing ways to make future turbines more reliable, tolerant of faults, and capable of diagnosing themselves.

The U.S. electric grid carries about 920 GW of capacity. The wind off the coasts of New England theoretically could yield a sizable fraction of that amount—perhaps 100 GW of capacity—said David Garman, DOE's assistant secretary for Energy Efficiency and Renewable Energy. Researchers estimate that this capacity could provide enough electricity to run about 40 million U.S. homes. With so much energy so near, NREL scientists are exploring new ways to exploit that resource, applying ideas that were unimagined a decade ago. "We can't let the projects drive the research," says Musial. "We want to get ahead of what's being done today, so new technology is available when the industry is ready."



Shown above is a concept for anchoring large wind turbines in deep water. On the opposite page, a 3.6-MW General Electric wind turbine stands in shallow water in an area off the coast of Ireland known as the Arklow Bank (opposite page). The first seven turbines in this proposed 200-turbine, 520-MW wind field started producing power in 2003. (Photo courtesy of GE Energy, © 2004, General Electric Company.)

### For More Information

Musial, W.; Butterfield, S. (2004). "Future for Offshore Wind Energy in the United States." Preprint. 16 pp.; NREL Report No. CP-500-36-313.

Web site for the European Wind Energy Association, accessed December 30, 2004. <http://www.ewea.org/>.

"Wind Farms off East Coast Could Yield 100 GW of Energy; DOE Official." *Inside Energy*; August 30, 2004; p. 15.



# Research Update

## Enhancing Geothermal Power

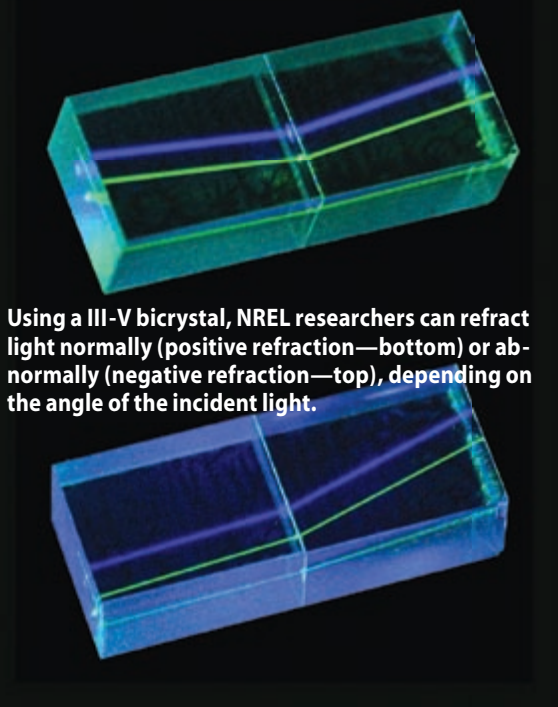
Producing power from geothermal energy resources is, in some ways, a remarkably successful endeavor. It is a clean source of power that produces very little carbon dioxide and almost no nitrous oxide or sulfur-bearing gases. Geothermal power plants have high capacity factors and average availabilities of 90% or more. And geothermal power production is a billion-dollar-a-year industry, producing nearly 20% of the nation's non-hydro renewable electric energy. Since 1970, geothermal power plant capacity has grown from 500 MW to more than 2,600 MW today.

But geothermal power production is currently limited to sites where geothermal energy reservoirs are relatively close to the surface. Because the power plant technology relies on extracting hot water from these reservoirs, they must also consist of fractured rock permeated with water, a geographic coincidence that occurs in limited locations in the West.

Given these limitations, how can the industry grow? The answer is to drill deeper to reach the geothermal heat and, when necessary, to add water and create new fractures. Such "enhanced geothermal systems," or EGS, can potentially expand the use of geothermal energy to any part of the country.

"It becomes almost an unlimited resource," says Gerry Nix, NREL's technology manager for Geothermal Technologies.

The main thrust of EGS is to inject high-pressure water into geothermal hot spots to open fissures that may be blocked with mineral deposits. It's a technique often used today by the oil and gas industry. At the Coso geothermal plant, about 100 miles north of



Using a III-V bicrystal, NREL researchers can refract light normally (positive refraction—bottom) or abnormally (negative refraction—top), depending on the angle of the incident light.

## Negative Refraction of Light

NREL physicists Yong Zhang, Brian Fluegel, and Angelo Mascarenhas have bent light the "wrong way," the first to do so using natural materials. In physics this is a pretty big deal. Why? Consider a stick in water. It appears bent where it enters the water. This is due to the phenomenon known as refraction. When light goes from one medium into another, it changes speed, causing it to alter direction. In refraction, the incident light and the refracted light are always on opposite sides of the normal, a line drawn perpendicular to the interface between the two materials. Thus it has always been.

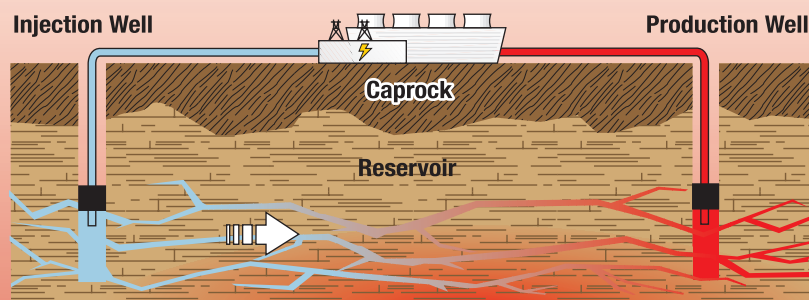
The ancient dictum that says light must be refracted to the opposite side of the normal was challenged in 1968 by Russian physicist V.G. Vaselago, who suggested that under special circumstances light could be "negatively refracted," or bent to remain on the same side of the normal. In the past couple of years, teams of scientists have begun to show that Vaselago may have been right.

They have designed special, elaborate configurations of "metamaterials" made of copper rings and wires and Teflon, which they have used to negatively refract narrow bands of microwaves. (A metamaterial is an artificially fabricated structure that exhibits properties not found in nature.)

NREL physicists have taken the demonstration a few steps further. Using "real" material—twinned bicrystals of a III-V semiconductor alloy (a twinned bicrystal is one in which two crystals intergrow and are mirror symmetrical about their interface)—they were able to attain negative refraction for visible light. More than that, they showed that, depending on the angle of incidence, they could get positive or negative refraction. What's more, they demonstrated that they could do the same thing for ballistic electrons as well as for light. And, finally, they showed that light could be refracted without losing energy or intensity (due to reflection), which is noteworthy in itself.

Can we harness this new capability? Perhaps. Although this is a new and fundamental discovery, we can already see possible uses in imaging, lens technology, data storage, semiconductor technology, and more. But uses inherent in the ability to steer and bend light, and to collimate electrons, will have to wait on more fundamental research and experimentation.

**In EGS, water is injected into a geothermal reservoir to promote fracturing. It is then circulated through the hot rock to heat the water and returned via a production well to produce geothermal electricity.**





Los Angeles, a project now under way is fracturing the existing reservoir to increase its size. The effort is expected to boost power production at Coso by 20 MW, to 260 MW total.

EGS also includes efforts to drill deeper at less cost and to convert the hot water into electricity more efficiently. As such, EGS is a graded approach to expanding the geothermal industry. By developing a "toolbox" of new techniques, the industry can gradually increase power production from existing geothermal reservoirs while expanding into areas that are currently beyond its reach. NREL is part of a virtual team spanning the DOE national laboratories that is developing this toolbox.

"NREL is helping to define the next generation of power plants, so we can efficiently convert the heat into power," says Nix. "We have assembled a group of experts to provide the planning, analysis, and integration needed for the scale of this research program."

By successfully developing and employing the EGS toolbox of techniques, DOE expects that the United States could increase its geothermal electric capacity to 20,000 MW by 2020.

## Measuring Minority-Carrier Lifetimes

An analysis technique developed at NREL offers a simple, effective way to test the performance of PV materials used to build solar cells. The technique—the Resonant-Coupled Photoconductive Decay System, or RC-PCD—offers a hands-off method to measure the lifetime of so-called "minority carriers" in PV materials.

A solar cell is made from semiconductor layers. One layer is engineered to be n-type, to have an excess of unbonded electrons as potential negative charge carriers. The other layer is prepared as p-type, to have an excess of free "holes" as potential positive charge carriers. Sandwiching the layers together forms a p/n junction with the free electrons and holes traveling across the junction to set up an electric field across the cell.

When light strikes either PV layer, the light energy frees negatively charged electrons within the material, which leaves holes where electrons use to be. Electrons freed by sunlight in p-type material are minority carriers; they tend to be propelled by the electric field across the junction into the n-type material where they migrate toward that end of the cell. Likewise, holes freed by sunlight in n-type material are minority carriers in that material; they are propelled by the electric field across the junction to the p-type material to migrate toward that end of the cell. It is this migration of minority carriers that creates the electric current and power.

Unfortunately, in many parts of a solar cell, the electrical field is too weak to whisk minority carriers off to their designated ends. Instead, the electrons and holes may wander randomly, possibly recombining with each other and wasting their energy as heat instead of producing power. Minority carriers that "live" longer have a greater chance of producing power, so PV materials should ideally have long minority-carrier lifetimes. Defects in the materials create stepping-stones that facilitate recombination, so minority-carrier lifetimes are also an indirect way to measure material defects.

The RC-PCD system, created by an NREL team led by Dick Ahrenkiel, measures minority-carrier lifetimes using a coil of wire. This coil, placed near the material, acts as an antenna, and a high-frequency signal pumped into it generates a low-energy microwave signal. Using electronic circuitry, the antenna can be tuned to perfectly transfer its energy to the material—a technique called resonance coupling.

The system uses laser pulses to generate electron-hole pairs in the material. The pairs

change the material's conductivity and cause it to respond differently to the antenna's signal, reflecting part of the signal back to the antenna. Ahrenkiel's team can detect that reflected signal and watch it drop off as the pairs recombine—a process called "photoconductive decay." By pulsing the laser, the system causes the photoconductive decay to occur repetitively. An oscilloscope averages the signals to create a smooth decay curve that provides an accurate measurement of the minority-carrier lifetime.

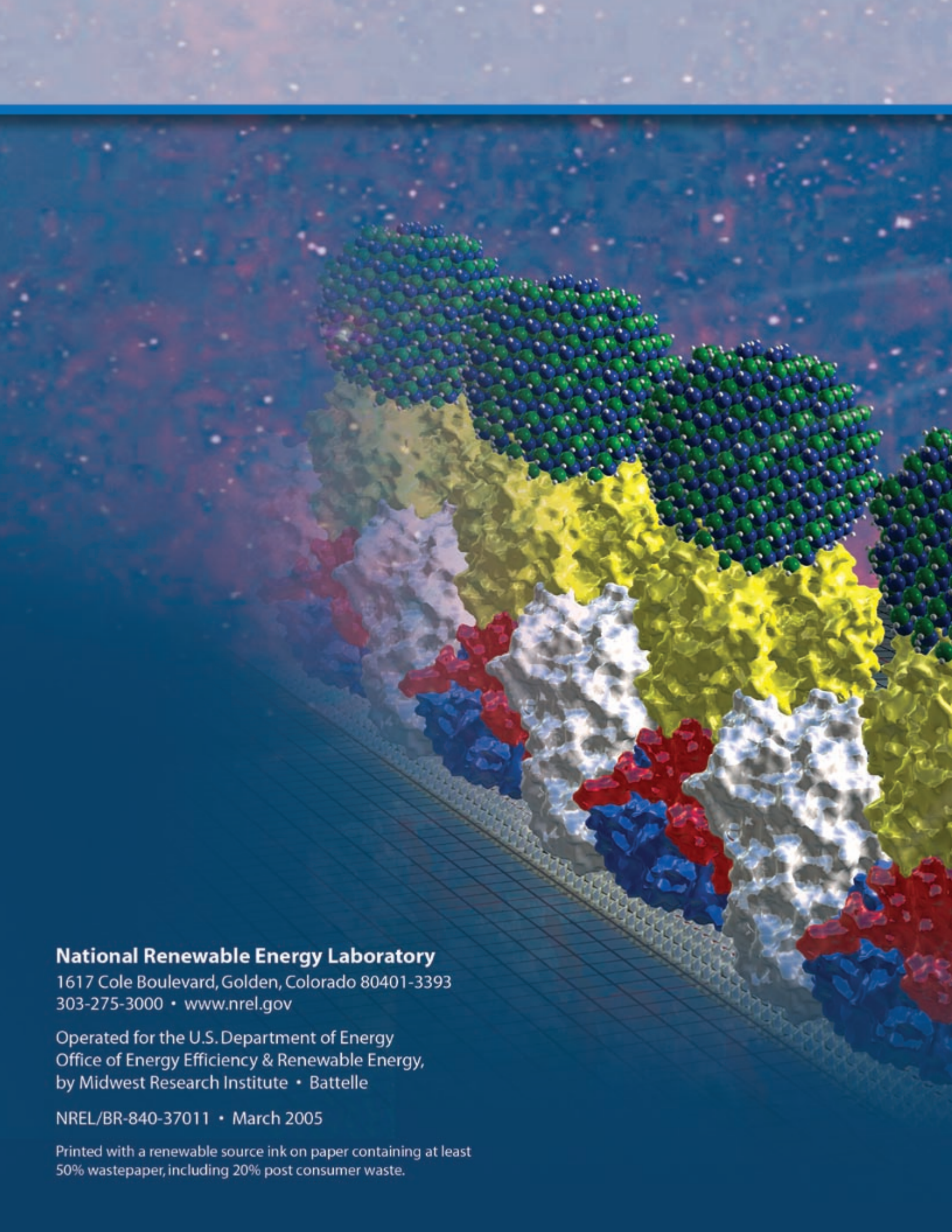
"We can do things here that nobody else can do," says Ahrenkiel. "It's become a standard in the PV program; we've run hundreds of samples through here. It has a lot of advantages over commercially available systems."

Those systems, mostly invented for the semiconductor industry, operate at higher frequencies that cannot penetrate into the depth of the material as the RC-PCD system can. That's fine for semiconductors, but unsatisfactory for thick solar cells, which depend on the entire thickness of the material to generate a current. The RC-PCD also offers other advantages. It has a greater dynamic range, is far more sensitive and accurate over that range, can measure lifetimes for a wider variety of materials and sample sizes, and has a greater ability to detect defects and their effect on lifetimes.

The system does have a drawback. It is limited to measuring lifetimes of 50 nanoseconds or longer, a limitation that some commercial devices can beat. To overcome that limitation, graduate student Jamiyana Dashdorj is inventing a new, better antenna. Ironically, software and electronics developed for the burgeoning cell phone industry are proving ideal for the task, so the cell phone technologies of today may help the solar cell industry invent the ideal energy source for tomorrow.

In the background is an early prototype of NREL's RC-PCD, a non-contact method that quickly and accurately measures minority-carrier lifetimes of photovoltaic and semiconductor materials. The latest version of the instrument (not shown) is far more compact and self-contained.





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